#### CHEMISTRY

# M. Sc. (Previous)

There shall be five papers in theory and three practical examinations separately as per following details:

Paper I: Symmetry & Spectroscopy 100 Marks Paper II: Inorganic Chemistry **≸** 100 Marks Paper III: Organic Chemistry 100 Marks Paper IV: Physical Chemistry 100 Marks Paper V: Special Topics in Inorganic Chemistry 100 Marks Practical: Inorganic Chemistry 75 Marks Practical: Organic Chemistry 100 Marks Practical: Physical Chemistry 75 Marks

# M. Sc. (Final) 2019-20 (w.c.f.)

There shall be five papers in theory and three practical examinations separately as per following details:

Paper I:	Inorganic Spectroscopy & Bio-inorganic	100 Marks
Paper II:	Organic Spectroscopy, Pericyclic & Photochemistry	100 Marks
Paper III:	Organic Synthesis	100 Marks
Paper IV:	Biomolecules	100 Marks
Paper V A:	Environmental & Analytical Chemistry	100 Marks
Paper V B:	Medicinal Chemistry	100 Marks
Paper V C:	Chemistry of Materials	100 Marks
Paper V D:	Polymers	100 Marks
Paper V E:	Reseaarch Aptitude in Chemistry	100 Marks
Practical:	Inorganic Chemistry	75 Marks
Practical:	Organic Chemistry	100 Marks
Practical:	Physical Chemistry	75 Marks

Note: 1. Paper V is elective. Student have to opt only one among paper VA- VE .

2. For elective paper to be taught minimum ten students should be enrolled.

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#### M.Sc. (Previous)

#### Paper I

#### Symmetry & Spectroscopy

- Symmetry: Symmetry elements, Symmetry operations, Symmetry point group, Identification of
  molecular point group, Molecules of low symmetry, high symmetry and special symmetry (C<sub>n</sub>,
  S<sub>n</sub>, D<sub>n</sub>, C<sub>nv</sub>, D<sub>nh</sub> only)
- 2. Group, Classes: Definition, multiplication table, group generating elements, subgroup, classes, derivation of matrices (C<sub>n</sub>, σ, i, S<sub>n</sub>), Direct product, Group multiplication basis, matrix representation, Character of an operation, orthogonality projection and shift operators, character table, orthogonality theorem, irreducible representation, Transformation matrices, structure of character table, determination of symmetry species for translations and rotations, construction of character table (C<sub>2v</sub>, C<sub>3v</sub>)
- Valence Bond Theory: Formation of hybrid orbitals of XY<sub>3</sub> (planar) XY<sub>4</sub> (T<sub>d</sub>, square planar).
   Symmetry of orbital, orbital symmetry properties, Projection to get symmetry orbital, projection operations, basis functions and hybrid orbitals with example
- 4. Molecular vibrations: Internal and symmetry coordinates, SALC's, Symmetric normal vibrations, mixing of linear coordinates in normal modes, determination of symmetry types of normal modes, determination of symmetry types of normal modes, analysis of vibration of 1, 2 dichloro ethylene.
- Unifying Principles: Electromagnetic radiation and its characteristics, Absorption, Emission spectroscopy, Born – Oppenheimer approximation, Rotational, Vibrational and electronic energy levels, Classification of spectra, Region of spectrum.
- 6. Infrared Spectroscopy: Linear harmonic oscillator, Vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential, Vibration rotation spectroscopy, P, Q, R branches, Breakdown of oppenheimer approximation, vibration of polyatomic molecules, selection rules, Group frequencies, Overtones, Hot bands, factors affecting the bond positions and intensities for IR region
- Normal Coordinate Analysis: Cartesian coordinate and internal coordinate methods applied to C<sub>2v</sub>(Sym XY<sub>2</sub>, ZXY<sub>2</sub>), C<sub>3v</sub>(XY<sub>3</sub>), T<sub>d</sub> (XY<sub>4</sub>) and O<sub>n</sub>(XY<sub>6</sub>) system, IR and Raman activity of some typical molecules (C<sub>2v</sub>, C<sub>3v</sub>, C<sub>4v</sub>, D<sub>2h</sub>, D<sub>3h</sub>, D<sub>4h</sub> point group)
- Raman Spectroscopy: Classical and quantum theories of Raman effect, Pure rotational, Vibrational and Vibrational – rotational Raman spectra, Selection rule, Mutual exclusion principle, Resonance Raman spectroscopy, CARS
- 9. Diffraction Techniques: -
- (A) X- ray Diffraction: General Features of diffraction, Powder X-ray diffraction, Single crystal X-ray diffraction: The technique, structure factor, phase problem, brief description of time resolved X-rays diffraction techniques.
- (B) Electron Diffraction: Scattering intensity vs scattering angle, Wierl equation, Measurement technique, Elucidation of structure of simple gas phase molecules, Low energy electron diffraction structure of surfaces
- (C) Neutron Diffraction: Brief introduction, difference with X-rays diffractions.

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#### M.Sc. (Previous)

#### Paper II

#### Inorganic Chemistry I

- Stereochemistry and bonding: VSEPR theory- stereochemical rules and explanation of the shapes of molecules and ions of nontransition element with 2-7 valence shell electron pairs, Walsh diagram (Tri and penta atomic molecules) dπ-pπ bonds, Bent rule, Energetics of hybridization
- Synthesis, Properties and Structures: Halides and oxides of nontransition elements, silicates
  and carbides, silicones, phosphazenes, sulphur- nitrogen compounds, Peroxo compounds of B,C
  and S, Oxyacids of N, P, S and Halogens, interhalogens, Pseudohalides, Noble gas compounds
- 3. Structures of 2 to 8 Coordinate Metal Complexes: Cation -anion ration in various polyhedral, hybrid orbitals and preferred conditions of formation of the complexes of following geometries: CN 2 Linear, CN 3 Trigonal planar, Trigonal pyramidal, CN 4 -Tetrahedral, Square planar, CN 5 Trigonal bipyramidal, Square pyramidal, pentagonal, CN 6 Octahedral, Trigonal prism, CN 7 Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism, CN 8- Cubic Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal and bicapped trigonal prism, Stereochemical non-rigidity in four to eight coordinate complexes
- 4. Stereoisomerism: Stereoisomerism in six coordinate octahedral complexes (Ma<sub>3</sub>bcd, Ma<sub>2</sub>bcde, Mabcdef and complexes containing bi and ter dentate ligands) intermolecular and intramolecular rearrangements (Bailar and Ray Dutta twist only), mechanism of racemisation in tris(chelate) octahedral complexes, Methods of resolution of optical isomers.
- 5A. Crystal Fields: Derivation of d orbital splitting patterns of ML<sub>2</sub>, ML<sub>3</sub>, ML<sub>5</sub> and ML<sub>7</sub> system (energy calculations are not required), the effect of weak field on.
- 5B. Metal ligand bonding: Limitation of CFT, Nephelauxetic series, Molecular orbital energy level diagram of octahedral, tetrahedral and square planar complex.
  - Metal Ligand Equilibria in solution: Stepwise and overall formation constants and their relations, factors affecting stability of metal complexes with reference to the nature of metal ions and ligands, Determination of stability constants by pH metric and spectroscopic methods.
  - 7. Kinetics and Mechanism
    - (A). Substitution Reactions: In octahedral Co(III) and Square planar Pt(II) complexes
    - (B). Electron Transfer Reactions: Mechanism of one electron reactions (inner and outer sphere mechanisms), factors affecting the rates of direct electron transfer reactions and the Marcus equation, two electron transfer reactions

#### 8. Electronic spectra of complexes

A. Energy levels in an atom: Relation between electronic configuration and energy terms, Hund's rules and ground state energy terms, inter electron repulsion parameter, variation of reaction B and C parameters in different transition series, spin orbit coupling parameters

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- B. Free ions in crystal fields: Effect of weak crystal field on free ion S, P, D, F and G terms in octahedral, square planar and tetrahedral symmetries, orgel diagrams, mixing of terms, medium and strong field approximation in on point group, transition from weak to strong field and correlation diagram for only d<sup>2</sup>case, Non crossing rule, Tanbe sugano diagrams.
- C. Interpretation of the spectra: of aqueous solution of [M(H<sub>2</sub>O)<sub>6</sub>]<sup>n+</sup>, calculation of Dq, B parameters, John Teller distortions and its effect on electronic spectra.
- 9. Magnetic Properties of Complexes: Dia, para, ferro and antiferromagnetism, quenching of orbital angular momentum by ligand, The magnetic properties of A, E and T terms.
- 10. Supramolecular Chemistry: Concept, molecular recognition, nomenclature, metallo -macrocyles as receptors, design of supramolecular through non covalent interaction and their application in transport process.

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#### M.Sc. (Previous)

#### Paper III

#### Organic Chemistry

- 1. Nature of bonding: Cross conjugation, Steric inhibition of resonance, aromaticity, antiaromaticity, huckel rule, energy level of  $\pi$  MOs, Homoaromaticity, PMO approach, alternate and nonalternate system, Aromaticity, generation and reactions of nonbenzonoids (tropolone, azulene, annulene, heteroannulene, ferrocene, fullerene)
- 2. Basic Principle: Potential energy diagram, Thermodynamic and kinetic requirement and control, methods of determining reaction mechanism, Labelling and kinetics isotope effect (Product analysis: kinetic and stereochemical studies), Solvent isotope effect, Hammond's postulate, Curtin Hammett principle, structural effects on reactivity, resonance, field effects, steric effects, Hamett equation and linear free energy relation (LFER), substituent and reaction constant, Taft treatment of polar and steric effects in aliphatic compounds (Taft equation), Transition states and intermediates, Generation, structure, stability and reactivity of carbocations, non classical carbocations, carbanions, carbenes, benzyne, nitrenes.
- 3. Stereochemistry: Stereochemistry with chiral centre: chirality, Polychiralcentre molecules, Threo erythro isomers, stereomerism with axial/ planar chirality and Helicity: Principle of axial and planar chirality, optical isomerism in the absence of chiral carbon (biphenyl, allenes, spiranes), optical activity due to intramolecular overcrowding, chirality due to helical shape, Absolute configuration (R/S, E/Z), Stereochemistry of compounds having S,N, P atoms, Geometrical isomerism of compounds having C=N, N=N bonds.

Topocity and Prostereoisomerism: Homotopic, enantiotopic and diastereotopic atoms, groups and faces, nomenclature and symbols

**Atropisomerism:** Conformational analysis of acyclic system, Interconversion of Fischer, Newmann and Sawhorse projection, its effect on reactivity (SN<sup>1</sup>, SN<sup>2</sup>, E<sup>1</sup>, E<sup>2</sup>) configuration, conformation and stability of cycloalkanes, mono and disubstituted cyclohexane, cyclohexenones, decalin, decalol

#### 4. Substitution Reaction

- (A) Aliphatic Nucleophilic Substitution:  $SN^1$ ,  $SN^2$ ,  $SN^i$ ,  $SN^2$ ,  $SN^i$ , mixed  $SN^1$  and  $SN^2$ , SET, factors (substrate structure, nucleophile leaving group solvent) affecting these substitution reactions, ambidentate nucleophile, Regioselectivity, competition between  $SN^1$  and  $SN^2$ , Nucleophilic substitution in bridged system phenonineun ion, norbornyl system, Neighbouring group participation (Ph,  $\pi$ ,  $\sigma$ , N, S, negatively charged oxygen), anchimeric assistance
- (B) . Aromatic Nucleophilic Subtitution: Aromatic SN¹ and SN², addition elimination (ipso) and elimination addition (benzyne) mechanism, S<sub>RN</sub>¹, effect of substrate structure, nucleophile, leaving group, von Richter, Smile rearrangement
- (C). Aliphatic Electrophilic Substitution: SE<sup>1</sup> and SE<sup>2</sup>, SET, SE accompanied by double bond shifts, Effect of substrate, leaving group and solvent polarity on reactivity
- (D). Aromatic Electrophilic Substitution: General view, energy profile, Arenium ion mechanism (ArS<sub>E</sub>), orientation and reactivity, o/p ratio and ipso substitution, Diazonium coupling, Vilsmeric reaction, Gattermann Koch reaction

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- 5. Free Radical Reactions: Types, generation, structure, state, radical effect, substitution mechanism at an aromatic substrate at a bridgehead, reactivity in the attacking radicals, effect of solvent on reactivity, Allylic halogenations (NBS), oxidation of aldehydes, autooxidation, Alkynes coupling and arylation of aromatic compounds by diazonium salts, Sandmayer reaction, Hunsdiecker reaction
- 6. Elimination Reaction: E<sup>1</sup>, E<sup>2</sup>, EkB, Factors affecting (substrate structure attacking base, leaving group, medium E<sup>1</sup>, E<sup>2</sup> and EKB), stereochemistry, spectrum orientation of double bond (Saytzelf vs Hofmann elimination), Mechanism and orientation of Pyrolytic syn elimination, chugaev, Hofmann, Competition with substitution reaction

#### 7. Addition Reaction:

- (A). Carbon Carbon bond: Mechanism, stereochemistry, electrophilic, nucleophilic, free radical addition, addition of halogen acid, 1,2 bishydroxylation, epoxidation, hydroboration, oxymercuration – demercuration, Addition to cyclopropane ring, hydrogenation of double bond, triplebond, aromatic ring, Michael addition, Robinson annulations, Regioselectivity, Chemoselectivity
- (B). Carbon heteroatom multiple bond addition: C=O bonds, cram rule, condensation reactions involving enolates Aldol (including directed aldol) stobbe, Claisen, Dieckmann, Mammich, Benzoin, Perkin, Knoevenagel, Darzen, Schmidt, Witting, Refermatsky, Esterification and hydrolysis of ester, evidence for tetrahedral intermediate in B<sub>AC</sub><sup>2</sup> and A<sub>AC</sub><sup>2</sup> mechanism, steric and electronic effects, A<sub>AC</sub> and other pathways involving to oxygen bond cleavage; Hydrolysis of amides, Amminolysis of esters, Cannizzaro reaction

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#### M.Sc. (Previous)

#### Paper IV

#### Physical Chemistry

#### 1. Quantum Chemistry:

- (A) Fundamentals: Introduction of classical mechanics and Quantum mechanics. Planck's quantum theory, Wave particle duality, Uncertainty principle, postulates of quantum mechanics, Schrödinger wave equation, its discussion for particle in a box (1D & 3D), the harmonic oscillator, the rigid rotor, the hydrogen atom.
- (B) Approximation methods: The variation method linear variation principle, Perturbation theory (first order and nondegenrate), application of both method to He atom
- (C) Angular Momentum: Ordinary, generalized, eigen functions, eigen values, operator using ladder operators, addition of angular momenta, spin, antisymmetry, Slater determinantal wave function, Pauli exclusion principle
- (D) Electronic Structure of Atoms: Electronic configuration, Rusell sounders terms and coupling schemes, Slatar Condon parameters, Term symbols and spectroscopic states, energies of the p<sup>n</sup> and d<sup>n</sup> configurations, magnetic effects, spin orbit coupling, Zeeman splitting, Self-consistent field method, Viral theorem
- (E) Born Oppenheimer approximation: Hydrogen molecule ion, LCAO, MO and VB treatment of the H<sub>2</sub>.
- (F) MOT: Huckel pi electron theory, bond order, charge density calculations, Application to ethylene, butadiene, benzene, cyclopropenyl radical, cyclobutadiene, Extended Huckel theory (introduction)

Forces and their role in chemical binding. Hybridization and valence MOs of H<sub>2</sub>O, NH<sub>3</sub> and CH<sub>4</sub>

## . 2. Thermodynamics

- (A). Classical: First law, relation between Cp & Cv enthalpies of physical and chemical changes, kirchoff equation, Joule Thomson effect, Second law. Entropy, Gibbs Helmholtz equation, Third law
- (B). Chemical Equilibrium: Free energy, entropy of mixing, partial molar quantities (free energy, volume, heat content), Gibbs Duhem equation, Equilibrium constant, van't Hoff equation, Fugacity and its determination
- (C). Phase Diagram: Phase rule, Phase diagram of one and two component systems.
- (D). Ideal and Non- ideal Solution: Excess function, activities, hydration number, activities in electrolytic solution, mean ionic activity coefficient, determination of activity
- (E). Non equilibrium Thermodynamics: Postulates, methodologies, linear laws, Gibbs equation, Onsagar reciprocal theory
- (F). Statistical Thermodynamics: Thermodynamic probability and entropy, concept of distribution, most probable distribution, Ensemble averaging, Maxwell Boltzmann distribution, postulates of canonical, grand canonical, microcanonical ensemble, Bose Einstein and Fermi Dirac statistics, Partition function, Translational, rotational, Vibrational and electronic partition function for diatomic molecules. Calculation of thermodynamic

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functions and equilibrium constant, theories of specific heat for solids, application of partition function

#### 3. Reaction Dynamics:

Methods of determining rate laws, mechanism of photochemical ( $H_2$ +  $Br_2$ ,  $H_2$ +  $Cl_2$ ), chain stopped ( $H_2$  equation +  $Br_2$ , decopposition of  $CH_3$ CHO, decoposition of  $C_2H_6$ ), oscillatory reaction, collision theory, steric factor, Absolute reaction rate theory, comparision of result with Eyring and Arhenius equation, steady state kinetics, kinetic and thermodynamic control of reactions, ionic reactions, kinetic salt effect, homogeneous catalysis, kinetics of enzyme reactions, heterogeneous catalysis, Fast reactions, luminescence and electron transfer process, flow technique, Relaxation method, flash photolysis, magnetic resonance method

- (A). Electrodynamics: Electrode kinetics, Electroosmosis (quantitative treatment), electrophoresis, streaming potential, electrical layer theories, Electrical double layer, electrode/ electrolyte interface,
  - (B). Electrolytic conductance and transference, Debye Huckel theory of strong electrolyte (DHO eqn), Debye Falkenhagen effect, Wein effect, activity coefficient, ionic strength, its effect on reaction rate, Debye Huckel theory of mean activity coefficient of strong electrolyte (DHLL)
  - (C). Electrochemical Cell Reactions: Galvanic cells, half reactions and reversible electrodes, single electrode potential, thermodynamics of reversible electrodes and cells, Nernst equation, Standard Electrode potential, Electrochemical series, EMF of Galvanic cells, activity and mean ionic activity of electrolytes, Concentration cell electrode and electrolyte, Electrolyte concentration cell with and without transference, Liquid junction potential, fuel cell primary and secondary fuel cells, batteries, application of emf measurement
  - (D). Electrolyte interface: Bjerrum theory of ion association in electrolyte solutions, Lippmann equation, determination of surface excess, structure of electrified interface, Guoy Chapman, Stern
  - (E). Electrodics: Buttler Volmer equation, Tafel equation
  - (F). Irreversible electrode process: Overvoltage, corrosion (mechanism, corrosion current, corrosion potential, electrochemical corrosion theory, estimation of corrosion rates prevention methods, polarization resistance, electrodeposition

#### 5. Surface Chemistry

- (A). Adsorption: Surface Tension, capillary action, Laplace equation, Kelvin equation, Gibbs adsorption isotherm, BET equation, Electri kinetic phenomenon
- (B). Micelles: Surface active agents, classification, micellization, hydrophobic interaction, CMC, factors affecting CMC, Counter ion binding to micelles, solubilization, microemulsion, reverse micelles
- (C). Macromolecules: Definition, types, electrically conducting, fire resistant, liquid crystal polymers, kinetics, mechanics, Molecular mass, number and mass average molecular mass, molecular mass determination, sedimentation

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#### M .Sc.(Previous)

#### Paper V

#### Special Topics In Inorganic Chemistry

- Metal Carbonyls: Preparation, Structure and properties of mononuclear and polynuclear metal carbonyls, Nature of M - C - O bonding, Vibrational spectra of metal carbonyl, Principle reaction types, Verities of CO bridging
- 2. Metal nitrosyls: bonding, structrure, Metal carbonyl- metal nitrosyl complex; Carbonyl metal
- Organometallics: Nomenclature, general characteristics, Major types of transition metal to carbon bonds excluding π - complex, Classification of organometallic compounds based on heptacity and polarity of M - C bond
- 4. Inorganic π-Acid ligands: O2, N2, nitrosyl; tertiary phosphine and arsines as ligands
- 5. Complexes of σ donor ligands: Transition metal alkenyls, alkynyls and carbines
- 6. Pi Complexes of unsaturated molecules: General methods of preparation, important reactions, with special reference to organic synthesis, bonding, structure of alkenes, alkynes, allyl, dienyl(cyclopentadienyl), trienyl(arenes) complexes, Structure and bonding in Zeise's salt, Ferrocene, Dibenzenechromium, Fluxional molecule
- 7. Transition Metal compounds with M H bond: Metal hydrides (Classical, non classical), Agostic interactions, Application of NMR in studying hydrido complex
- Metal Clusters and M H bond: M M multiple bonds contain binuclear and trinuclear, tetranuclear and octahedral clusters, synthesis and bonding in clusters, metal carbonyl halides, Chalcogenide clusters
- 9. Metal alkoxides: Preparation, Properties, Structure, Industrial application
- 10. Organometallic Catalyst: General ideal of important catalytic steps, Coordinate Unsaturation, Reaction of coordinated ligands and coordinated molecular oxygen, Template synthesis, Oxidative addition, Reductive elimination and inigration (insertion) reactions
- Macrocyclic Complex: Types of macrocyclic ligands, design and synthesis by coordination template effect, di and polynuclear macrocyclic complexes, Application of macrocyclic complexes
- Polyhedral Boranes: Higher boranes, Carboranes, metalloboranes, metallocarboranes, Structure and bonding in the light of Wade's and Jemmi's Rule
- 13. Isopoly and Heteropoly Acids and Salts: Synthesis, Structure, Principles with reference to those of V, Nb, Ta, Cr, Mo, W
- 14. between main group and Organometallic Chemistry: Isolobal concept (Hofmann) in Organometallic and metal cluster chemistry.

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# M.Sc. (Previous) Inorganic Chemistry Practical

# 1. Inorganic Mixture Analysis

Qualitative analysis of an inorganic mixture of seven radicals including one rare elements Tl, W, Se, Mo, Te, V, Be, U, Ti, Zr, Th, Ce and Li. Semi - micro analysis is to be done. Mixture can have insoluble substances, interfering anions and combination of anions.

- 2. Either both gravimetric or one gravimetric and other volumetric estimation of two metal ions from following mixtures
  - Cu2+ and Ni2+ (i)
  - Cu2+ and Zn2+ (ii)
- 3. Chromatographic separation of metal ion given in any one of the following combinations
  - Pb2+, Ag+, Hg22+ (i)
  - Co<sup>2+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup> (ii)
  - (iii) Fe<sup>3+</sup>, Cr<sup>3+</sup>, Al<sup>3+</sup>
  - Ba<sup>2+</sup>, Sr<sup>2+</sup>, Ca<sup>2+</sup> (iv)
  - Pb2+, Cd2+ (v)

#### System of Marking

Duration: 12h (2 days)		M.M: 75
Exercise 1: Inorganic Mixture analysis (seven radicals)		21
Exercise 2: Estimation		30
Exercise 3: Chromatographic Separation		09
Viva- voce		10
Record	,	05

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# M.Sc. (Previous) Organic Chemistry Practical

# 1. Qualitative analysis

Separation, purification and identification of components of binary organic mixture (two solids or one liquid and one solid). Systematic analysis of each components leading to their final identification laying emphasis or solubility, element detection, melting point, boiling point determination, ignition test, unsaturation test, functional group test and preparation of suitable derivative.

#### 2. Organic Synthesis

Two step simple preparation

(i)	Aniline	 sym-Tribromoaniline
(ii)	Chlorobenzene	 2,4 - Dinitrophenylhydrazine
(iii)	Aniline	 p - Nitroacetanilide

# System of Marking

Duration: 12h (2 days)	M.M: 100
Exercise 1: Binary organic mixture analysis	30
Exercise 2: Any one organic synthesis	30
Viva- voce	10
Record	05
Tour / Seminar / Project work	25

Report of tour / seminar/ project work must be submitted in hard copy.

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## M.Sc. (Previous) Physical Chemistry Practical

#### Section A

#### **Chemical Kinetics**

- 1. Kinetics of ester (ethyl acetate) hydrolysis in presence of acid
- 2. Kinetics of ester (ethyl acetate) hydrolysis in presence of alkali (NaOH)
- To compare the strength of HCl and H<sub>2</sub>SO<sub>4</sub> by studying the kinetics of hydrolysis of ethyl
  acetate.
- 4. Kinetics of acetone and I2
- 5. Kinetics of KBrO<sub>3</sub>/KI
- 6. Kinetics of H2O2/ HI
- 7. Kinetics of Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub>/ HCl
- 8. Kinetics of K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>/ KI

#### Section B

#### Thermochemistry

1. To determine the enthalpy of ionization of acetic acid

#### Solubility

- 2. To determine the solubility of a salt by gravimetric method.
- 3. To determine the solubility of a organic acid by titration method.
- 4. To determine the heat of solution of an organic salt by solubility method.
- To determine the solubility of benzoic acid in water at different temperatures and calculate heat of solution.
- 6. To draw the solubility curve for water acetic acid chloroform system.
- To determine the solubility of salicylic acid in water at different temperatures and calculate heat of solution.

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#### Electrochemistry

8. To determine solubility product of AgCl from E.M.F. measurement.

### Section C

## Colloidal and Surface Chemistry

- To determine the adsorption of aq. acetic acid by activated charcoal and study the adsorption (Freundlich isotherm)
- 2. To study the adsorption of oxalic acid on charcoal and draw the Freundlich isotherm.
- 3. To prepare As<sub>2</sub>O<sub>3</sub> and Fe(OH)<sub>2</sub> solution.

#### Distribution Law

- 4. To determine the distribution coefficient of I2 between H2O and CCl4
- 5. To determine the distribution coefficient of  $C_6H_5COOH$  between  $H_2O$  and  $C_6H_6$
- 6. To determine the distribution coefficient of  $CH_3COOH$  between  $H_2O$  and  $C_6H_6$
- To determine the equilibrium constant of the reaction (KI + I<sub>2</sub> 

  KI<sub>3</sub>) and formula
  of the complex formed between the cupric ion and ammonia by distribution method.

#### System of Marking

Duration: 12h (2 days)	M.M: 75	M.M: 75	
Exercise 1: Any one experiment from section A	20		
Exercise 2: Any one experiment from section B	20		
Exercise 3: Any one experiment from section C	. 20		
Viva- voce	10		
Record	05		

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## M.Sc. (Previous) Physical Chemistry Practical

#### Section A

#### Chemical Kinetics

- 1. Kinetics of ester (ethyl acetate) hydrolysis in presence of acid
- 2. Kinetics of ester (ethyl acetate) hydrolysis in presence of alkali (NaOH)
- To compare the strength of HCl and H<sub>2</sub>SO<sub>4</sub> by studying the kinetics of hydrolysis of ethyl
  acetate.
- 4. Kinetics of acetone and I2
- 5. Kinetics of KBrO<sub>3</sub>/KI
- 6. Kinetics of H<sub>2</sub>O<sub>2</sub>/ HI
- 7. Kinetics of Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub>/ HCl
- 8. Kinetics of K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>/KI

#### Section B

#### Thermochemistry

1. To determine the enthalpy of ionization of acetic acid

### Solubility

- 2. To determine the solubility of a salt by gravimetric method.
- 3. To determine the solubility of a organic acid by titration method.
- 4. To determine the heat of solution of an organic salt by solubility method.
- To determine the solubility of benzoic acid in water at different temperatures and calculate heat of solution.
- 6. To draw the solubility curve for water acetic acid chloroform system.
- To determine the solubility of salicylic acid in water at different temperatures and calculate heat of solution.

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#### Paper I

#### Inorganic Spectroscopy & Bioinorganic

Infrared and Raman Spectroscopy: Comparison of both, Application of Vibrational spectroscopy in determining symmetry and shapes of simple AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub> molecules, Mode of bonding of ambidentate ligands (SCN, NO<sub>3</sub>, SO<sub>4</sub><sup>2</sup>, NH<sub>2</sub>CONH<sub>2</sub>, en, diketanato), Metal ligand vibrations, Resonance Raman spectroscopy in study of active sites of metalloproteins, Application of IR and Raman spectroscopy in structural elucidation of simple inorganic and coordination compounds.

2. NMR spectroscopy: Structural application in <sup>1</sup>H NMR, <sup>13</sup>C NMR, <sup>1</sup>H NMR of paramagnetic substances, Lanthanide shift reagents, contact and pseudo contact shift, factors affecting nuclear relaxation, An overview of NMR of metal nuclides <sup>195</sup>Pt, <sup>119</sup>Sn NMR, use of chemicals as NMR auxiliary reagents (shift reagent, relaxation reagent), spin – spin coupling, Bloch equation, Line width and relaxation process, Application of chemical shift and coupling constant in structural determination of inorganic molecule, Application of contact shift in structural studies of

paramagnetic complexes, NMR studies of fluxional molecules.

3. ESR spectroscopy: Basic principles, Hyperfine splitting (Isotopic system), g value and factors affecting thereof, spin polarization for atoms and transition metal ions, interactions affecting electron energies in paramagnetic complexes (zero – field splitting, Kramer's degeneracy), Electron – electron interactions, Anisotropic effect (g – value, hyperfine couplings), Spin Hamiltonian, Spin densities, McConnell relationship, EPR of triplet states, structural application to transition metal complexes (having one unpaired electron), biological system, inorganic free radicals (PH<sub>4</sub>, F<sub>2</sub>, BH<sub>3</sub>), CIDNP

4. Mössbauer Spectroscopy: Basic principle, condition for it, spectral parameters (isomer shift, electric qudrepole interactions, magnetic interactions), Temperature dependent effects, Structural application for Fe<sup>2+</sup> and Fe<sup>3+</sup>, Sn<sup>2+</sup> and Sn<sup>4+</sup> complexes (nature of M-L bond, coordination structure), Detection of oxidation state and inequivalent mössbauer atoms; Spectrum display

5. Mass spectroscopy: Structural application

6. Role of Metal ions: Essential and trace metal ion

Role of alkaline earth metal ions in biological system, Catalysis of phosphate transfer by Mg<sup>2+</sup> ion, ubiquitous regulatory role of Ca<sup>2+</sup> in muscle contraction,

Metal ion storage and transport (Na, K, Ca, Mg, Fe, Cu, Zn), Ferritin Transferrin

Metal deficiency and disease

Toxic effects of metals and its curve by chelating agents, Pharmacological activity and metal chelates, Metals used for diagnosis and chemotherapy, anticancer drug, Carcinogenic metals, carcinogenic and carcinostatic ligands.

 Bioenergetics: Chlorophylls, PS I, PS II in cleavage of water, Glycolysis, Citric acid cycle, Oxidative phosphorylation, phosphorolysis and transport through membrane, Glucose storage, Metal complexes in transmission of energy, Oxidation of glucose and role of phosphate

8. Metalloenzymes: Function, structure, bonding and stereochemistry of the active site of

- (i) Natural dioxygen carriers: Haemoglobin, myoglobin, hemerythrin, hemocyanin
- (ii) Electron Transport: Iron sulphur protein Rubredoxin, Ferredoxin, Cytochromes (types a, b and c)

(iii) Redox enzymes:

(a) Mo containing: Nitrogenase, Xanthine oxidase, Sulphite oxidase, Nitrate reductase

(b) Fe containing: Cyt c oxidase, Catalases Peroxidases

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(c) Cu containing: Superoxide dismutase (SOD), Bovine superoxide dismutase (BOD), Ascorbic acid oxidase

(d) Zn containing: Carboxypeptidase A &B, Carbonic anhydrase, Urease

(e) Co containing: Vitamin B 6, Vitamin B12

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#### Paper II

#### Organic Spectroscopy, Pericyclic & Photochemistry

- Uv- visible Spectroscopy: Various electronic transitions (185 180 nm), Beer Lambert law, Chromophores, Auxochromes, Effect of solvent on electronic transitions, Red shift, Blue shift, Woodward's rule for conjugated cyclic and acyclic dienes, α, β- unsaturated carbonyl compounds, Absorption in aromatic compounds (substituted benzene, naphthalene and anthracene), Uv bands for carbonyl compounds, unsaturated carbonyl compounds, Heterocylces, steric effect in biphenyl
- 2. Infrared Spectroscopy: Vibration modes and bond stretching absorption by common function groups (alkanes, olefins, alkynes, aromatic hydrocarbons, alcohols, ketones, phenols, alkyl amines), Detailed study of Vibrational frequency of carbonyl compounds (ketones, aldehydes, esters, amides, carboxylic acids, acid anhydrides, lactones, lactams, conjugated carbonyls), effect of hydrogen bonding and solvent effect on Vibrational frequency, Electronic and steric effects, Fingerprint region, Interpretation of IR spectra, Instrumentation and sample handling, FTIR, IR of gaseous, solid, polymeric materials.
- 3. Proton Magnetic Resonance Spectroscopy: Spinning nuclei, Nuclear spin, nuclear resonance, saturation, chemical shift, its measurement, factors affecting it, Anisotropic effect, shielding mechanism, spin spin coupling, coupling constant, simple, virtual and complex coupling, chemical and magnetic equivalence, first and non first order spectra, Analysis of AB, AMX and ABX system, simplification of complex spectra, NOE, Deuterium exchange, Hindered rotation and rate process, NMR studies of <sup>19</sup>F, <sup>31</sup>P, Instrumentation, FTNMR, its advantage, Interpretation of <sup>1</sup>H NMR spectra, Application in structure elucidation
- 4. Carbon Magnetic Resonance Spectroscopy: Introduction, Peak assignment, chemical shift, <sup>13</sup>C <sup>1</sup>H coupling, off resonance, decoupling, deuterium, fluorine and phosphorous coupling DEPT, 2DNMR: COSY, NOESY, NETCOR, Application to simple organic molecule
- 5. ESR Spectrometry: Application to methyl, naphthalene, benzene free radical
- 6. Mass Spectrometry: Measurement technique (EI, CI, FD and FAB), Ion production, factors affecting fragmentation, Group metastable peak, Ion analysis, Molecular base and molecular ion, Ion abundance, factors affecting non abundance, Mc Lafferty rearrangements, reto Deils Alder Fragmentation, Nitrogen rule, Determination of molecular composition, Mass. Spectral fragmentation of organic compound, common functional group with reference to their structure determination, Interpretation of mass spectra, High resolution mass spectrometry
- 7. Solution of structural problems by combined application of Uv, IR, NMR (<sup>1</sup>H, <sup>13</sup>C) and mass spectrometry
- 8. Pericyclic Reactions:

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- (A) Basic concepts, classifications, characteristics, conservation of MO symmetry, FO of ethylene, 1-3 butadiene, 1,3,5 hexatriene, allyl system, woodward, Hoffmann rule for correlation diagram, FMO & PMO approach to study of
- (B). Electrocyclic reactions: Linear conjugated 4n, 4n+2, allyl system
- (C). Cycloaddition: [2+2], [4+2] system, [2+2] addition of ketene 1, 3 dipolar cycloaddition
- (D). Sigmatropic: [1, 3], [1, 5], [3, 3], [5, 5] Group transfer reaction suprafacial, antarafacial shift of H, Sigmatropic shift involving carbon moieties, clausien, cope rearrangement, Fluxional tautomerism, Aza cope rearrangement, Ene reaction, Chelotropic reaction, Prototropic reaction
- Photochemistry: Electronically excited states, spin multiplicity, Jablonski diagram, ISC
   (A). Photochemistry of alkenes: Geometrical isomerisation, cyclisation, dimerisation, di pi methane rearrangement, H abstraction addition, acetylene dimerisation, photochemistry of diene,

1,3 - butadiene, [2+2] addition reading to cage structure

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(B). Photochemistry of Carbonyls: Reduction, Norrish I cleavage of acyclic, cyclic,  $\alpha$ ,  $\beta$  and  $\beta$ ,  $\gamma$  unsaturated carbonyl compounds, Photochemistry of Norrish II cleavage, Paterno Buchi reaction intra and inter molecular H abstraction, rearrangement of  $\alpha$ ,  $\beta$  unsaturated ketones cyclohexadienones, Photoenolization, Photocycloaddition of ketones with unsaturated compound, photodimerisation of (enones),  $\alpha$ ,  $\beta$  unsaturated ketones, rearrangement of enones, dienones photochemistry of p – beinzoquinones,

(C). Photochemistry of aromatics: Ring isomerisation, Excited state of benzene and its 1, 2, 1,3 shifts, photo Fries rearrangement (of anilide), cylisation reactions, Skeletol isomerism, Dewar Prismane isomerisation of disubstituted benzene, Photo substitution reaction of benzene,

Photolysis of nitride ester

(D). Photochemical Rearrangements: Sommlet Hauser, Favorskii, Hofmann - Loffler Freytag,

Barton, Shapiro

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## M.Sc.(Final) Paper III **Organic Synthesis**

 Molecular Rearrangments: Pinacol – Pinacolone, Wagner Meerwin, Demjanov ring expansion, Dienone - Phenol, Benzil - binzilic acid, Wolf, Hoffmann, Curtius, Lossen, Schmidt, Beckmann, Baveyer Villiger, Stevens, Witting, Neber, Amino ketone, Benzidine

2. Selective Name Reactions: Stark enamine, Chichibabin, Mamrich, Birch reduction, Heek,

Suzuki, Mukaiyama, Woodward & Pervost hydroxylation, Peterson synthesis

3. (A) Oxidation: Different oxidative processes, Hydrocarbons - alkenes, aromatic ring, saturated C- H groups (activated and unactivated) Alcohols, diols, aldehydes, ketones, carboxylic acids, amines, hydrazines, sulphides

- (B). Reduction: Different reductive process, Hydrocarbon alkanes, alkenes, alkynes, aromatic rings, carbonyls - aldehyde, ketones, acids, acid derivatives, eposixides, hydrogenolysis
- Reagents: LiAlH<sub>4</sub>, NaBH<sub>4</sub>, SnBu<sub>3</sub>H, RhCl (PPh<sub>3</sub>)<sub>3</sub>, IC<sub>6</sub>H<sub>5</sub>(OAc)<sub>2</sub>, SeO<sub>2</sub>, RuO<sub>4</sub>, OsO<sub>4</sub>, RCO<sub>3</sub>H, HIO<sub>4</sub>, Pb(OAc)<sub>4</sub>, CH<sub>2</sub>N<sub>2</sub>, NBS, R<sub>2</sub>CuLi, LDA, DCC, 1,3 - dithiane (reactivity umpolung), Me<sub>3</sub>SI, Baker's yeast, organophosphorous compounds, yields (S,N, P), Phase transfer catalyst, quaternary ammonium and phosphonium salts, crown ethers, Merrified resins, DDQ, Jone's reagent, Tl(NO<sub>3</sub>)<sub>3</sub>, DIBAL, B<sub>2</sub>H<sub>6</sub>, di – isoamylborane, 9 – BBN

5. Organometallic Catalysts: Olefin hydrogenation (Wilkinson catalyst), Carbonylation of methanol to acetic acid (Monsanto process), Oxo process; Pd catalysed oxidation of ethylene (Wacker process), Olefin polymerization (Monsanto process), Fisher Tropsch process

6. Asymmetric Synthesis: Stereospecific, stereoselective synthesis, Enzymatic and catalytic nexus. Enantioselective synthesis with chiral non racemic and catalysts, hydroboration with chiral boranes(I<sub>PC</sub>BH<sub>2</sub>), (A<sub>Pc</sub>)<sub>21</sub>BH, carbonyl group reductions and chiral complex hydride (BINAL-H), Chiral oxazaberlidines, Diastereoselective synthesis, Asymmetric synthesis involving chiral, auxillary chiral reagent and chiral catalysis, methods of resolution, enantiomeric excess i.e; quasiracemate and optical purity

7. Green Chemistry: Basic principle, microwave induced organic synthesis, Combinatorial chemistry

8. Retrosynthetic Analysis: Synthon, synthetic equivalent, one group C-X and two group C-X disconn7. ection, Disconnection (C-C, C-S,C-O) bonds, FGI, Chemioselectivity, Cyclisation reactions, synthetic strategy for formation of C-C, C-N, C- halogen bonds. Reversal of polarity, Amine synthesis, multistep synthesis

Protection: Principles, deprotection of alcohols, thiols, 1,2 and 1,3- diols, amines, carbonyls and carboxyl groups in organic synthesis.

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# M.Sc.(Final) Paper IV BIOMOLECULES

1. Alkaloids: Definition, Nomenclature, Classification based on N- heterocyclic ring and biosynthesis, Physiological action, General method of structure elucidation, Degradation, Role of alkaloids in plants, Structure, Stereochemistry and synthesis: Nicotine, Quinine, Marphine (Retrosynthesis also), Ephedring, Connine, Atropine, Reserpine (Retrosynthesis also)

Terpenoids: Classification, General methods of structure elucidation, isoprene rule, structure, stereochemistry, synthesis: Camphor (Retrosynthesis also), Abietic acid, Squalene, α - Pinene, α - Cadinene, Citral, α - Terpenol, Menthol, Farnesol, Santonin, β - Carotene, Taxol (synthesis only),

Longifolene ((Retrosynthesis also)

 Steroids: Basic skeleton, Diel's hydrocarbon, nomenclature, structure, stereochemistry, synthesis: Cholesterol, Bile acid
 Note: In case of cholesterol questions will be asked only related to determination of ring system,

position of hydroxylic group, angular methyl group, double bond, nature and position of side

chain)

Prostaglandin: Occurrence, nomenclature, classification, physiological effects, synthesis: PGE<sub>2</sub> and PGE<sub>2a</sub>, Thromboxanes, approaches to prostaglandin synthesis: cyclohexane precursors (Woodward synthesis of PGE<sub>2a</sub>), Bicyclopentane precursors (Coxy's synthesis of PGE and PGF)

5. Proteins: Amino acids, polypeptide, structure of protein, Ramchandran plot

6. Nuclic acids: General structure of RNA and DNA

7. Carbohydrates: Conformation of sugars, structure, function, configuration of lactose, maltose, cellobiose, sucrose, cellulose, starch, glycogen

8. Heterocycles: Nomenclature of one, two, three heteroatoms containing heterocycles: Chemistry of azoles (oxa / thia / pyrazole, immidazole, thia / oxadiazole), pyrazine, pyrimidine, pyridazine

9. Biosynthesis: Acetate hypothesis, poly – β – keto acid, their aldol type cyclisation, metaorientation of hydroxyl group in naturally occurring phenols, biogenesis of fatty acids, malonic acid from acetyl coenzyme A, biogenesis of mono, sesqui, di, tri terpenes, skimic acid pathway for biogenesis of aromatic ring, general biogenesis of alkaloids.

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#### Paper VA

#### **Environmental & Analytical Chemistry**

- 1. Basics of environment: Concept, scope of environmental chemistry, terminology and nomenclature, Natural cycles (hydrological, oxygen, nitrogen, phosphorus and sulphur).
- 2. Atmosphere: Regions, reactions, Earth radiation balance, Particle ions and radicals present, Stratosphere, ozone layer, ozone layer depletion, Green House effect, Global warming, El-nino
  - Air pollution: Air pollutants (source, classification, sampling, monitoring), Particulates, Aerosols, SOx, NOx, COx, Hydrocarbon emission, Photochemical smog, Autoexhausts, Acid rain, Air quality standards
- 3. Hydrosphere: Chemical composition of waterbodies: lakes, streams, rivers, wet lands, complexation in natural and waste water, microorganism in aquatic chemical reactions, Eutrophication, Recycle of waste water, Sewage treatment, water reuse in industry and agriculture, microbiologically inediated redox reactions, Nitrogen transformation by bacteria Water pollution: Water pollutants, Water quality parameters, Standard physical and chemical parameters, DO, BOD, COD, TOC, TN, TS, TP, TC, chemical specification
- 4. Environmental Toxicology: Chemical solutions to environmental problems, Biodegradability, principles of decomposition, Better industrial process, Bhopal gas tragedy, Chemobyl, Three mile island, Sewozo and Minimata disaster.
- 5. Chemical Toxicology: Toxic chemicals in the environment, impact of toxic chemicals on enzymes, Biochemical effect of As, Cd, Pb, Hg, CO, NOx, SOx,O3, PAN, cyanide, pesticides, insecticides, carcinogens
- 6. Data Analysis: Systematic and random errors, Accuracy and precision and ways of its expression, Fitting data to a straight line, Normal error curve and its equation, Propogation of errors, Standard tests, Test of significance, F-test, student - t- test, Q-test, Chi- test, Correlation test, distribution normalcy test, confidence limit of mean, comparison of two standard value, comparision of standard deviation and average deviation, comparision of mean with true value, significant figures, Rounding of figures, Regression analysis ( least square method for linear plots), Rejection of observations, Statistics of sampling and detection limit evaluation
- 7. Electroanalytical Techniques: Conductometric, Polarographic (Limiting current density, Dropping mercury electrode, Jlkovie equation, Holf wave potential), Voltametry, Cyclic voltametry, Anodic stripping voltametry, Potentiometry, Amperometry, Ion selective electrodes, Coulometric
- 8. Thermoanalytical Techniques: TGA, DTA, DSC
- Spectroanalytical Techniques: Nephleometry, Turbidimetry
- 10. Separation Techniques: Distribution law: Principles and application of solvent extraction, Chromatography: Adsorbtion, Partition, Ion exchange, Size exclusion chromatography, Electrophoresis

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#### Paper VB

#### Medicinal Chemistry

1. Drug Design: Development of new drugs, Structure activity relationship (Structure activity relationship (SAR), Factors affecting bioactivity, isomerism, bio – isomerism, spatial considerations, Theories of drug activity, Occupancy theory, rate theory, induced fit theory, Quantitative structure activity relationship; History and development of QSAR concepts of drug receptors (Receptor site theory), elementary treatment of drug receptor interactions, Introduction to combination synthesis in drug discovery, Physico – chemical parameters, Lipophilicity, partition – coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potential, Generic medicines difference drug and medicine.

2. : Synthesis of penicillin-G, penicillin V, ampicillin, chlorounphenicol, Streptomycin, Cephalosporin C, Tetracycline

3. Vitamins: Thiamine (B<sub>1</sub>), Riboflavin (B<sub>2</sub>), Pantothenic acid (B<sub>3</sub>), Niacin (B<sub>5</sub>), Pyridoxine (B<sub>6</sub>), Ascorbic acid(C, C<sub>1</sub>), Calciferol (D)

Tocoferol (E: a, β, γ, δ), Ergosterol (K<sub>1</sub>, K<sub>2</sub>), Bioten (H)

· Chemistry and Physiological function

Retrosynthetic analysis of only calciferol

4. Harmones: Structure and function

Steroidal: Androsterone, Testesterone, Estrone (including relationship to estradiol), Progestrone, Aldosterone, Estrogen, Androgen,

Nonsteroidal: Theroxine, Andrenaline

Insect: Pheromones

Juvenile Plant: Gibbreluis

 Antineoplastic Drugs: Introduction, Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer, Mention of carcinolytic antibiotics and initopic inhibitors, Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, amustards and 6-mercaptopurine products, Nitrogen mustards

 Cardiovascular Drugs: Cardiovascular diseases, Drug inhibition of peripheral sympathetic function, Direct acting arteriolar dilators, Synthesis of amyl nitrate, hydrolaxine verapamil,

methyldopa and diazoxide propanol

7. Local Anti – infective Drugs: Antitubercular drugs and antimalarial drugs: Introduction and general mode of action, synthesis of sulphonamides, ciprofloxaction, norflocation, dapsone amino salicylic acid, ethionamide, ethambutal, griseofulvin, 4 – aminoquiooline derivatives, chloroquin, santoquine, camaquine, 8- aminoquinoline, primaquine, PAS, Thiosemicarbazones, hydrazides and thiocarbamlids

 (A). Psychoactive Drugs: CNS depressants, general anaesthetics, hypnotics, sedatives, antianxiety drugs, benzodiazipies mental diseases, Antipsychotic drugs, Synthesis of diazepam, alprazilam trimethadione barbiturates and glutethimide Reserpine, Promazine,

chloroopromazine, mepazine

(B). Antihistaminic drugs: Anatazotine diphenhydroamins

Sulpha drugs: Sulphanilamide derivatives, sulphathiazoles, sulphathabidine, sulphasuccidine, sulphaguamidine, sulphadiazine

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## (C). Anti HIV drug: Crixivan

9. Structure based drug classification: Drug based on a

- (i) Substituted benzene ring: Chloramphenical, salmeterol, Talazamide, dichlophenac, tiapamil, intryptiline
- (ii) Five membered heterocycles: Tolmetin, Spiralpril, oxaprozine, sulconazole, nizatidine, imolammine, isobuzole
- (iii) Six membered heterocycles: Warfarin, quinine, norfloxacin, ciprofloxacin, methylclothiazide, citrine, terfenadine
- (iv) Seven membered heterocyclic ring fused to benzene: Chlordiazepoxide, diazepam, diltiazem

(v) Heterocycles fused to two benzene rings: Quinacrine, tacrine

(vi) Five membered heterocycles fused to six membered rings: Acyclovir, methotrexate

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M.Sc. (Final) PAPER &C

Chemistry of Materials 60 Hrs (2 Hrs/week)

# Chemistry of Materials

5 Hrs

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VII

Multiphase Materials Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

# Glasses, Ceramics, Composites and Nanomaterials

5 Hrs

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and

Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

# Thin Films and Langmuir -Blodgett Films

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

# Liquid Crystals

10 Hrs

Mesmorphie behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nomatics, chiral nematics, molecular errangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

# Polymeric Materials

5 Hrs

Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.

#### Ionic Conductors VI

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Fronkel); yactancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors

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Chemistry

# VII High Tc Materials

10 Hrs

Defect perovskites, high T<sub>c</sub> superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high T<sub>c</sub> materials, applications of high T<sub>c</sub> materials.

# VIII Materials for Solid State Devices

3 Hrs

Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures; optical properties.

#### Organic Solids, Fullerenes, Molecular Devices IX

9 Hrs

Conducting organics, organic superconductors, magnetism in organic materials.

Fullerenes -doped, fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches -sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order - molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

# **Books Suggested**

- Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College. 1
- Material Science and Engineering, An Introduction, W.D. Callister, Wiloy. 2
- Principles of the Solid State, H.V. Keer, Wiley Eastern. 3.
- Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS 4.
- Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley. 5.
- Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag. 6.

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**Polymers** 

Polymers

60 Hrs (2 Hrs/week)

8 Hrs

Basics

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-lonic and co-ordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

# Polymer Characterization

14 Hrs

Polydispersion-average molecular weight concept. Number, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscocity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymerschemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

#### Structure and Properties 111

14 Hrs

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point Tm - molting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

#### Polymer Processing IV

12 Hrs

Plastics, clastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, toaming, reinforcing and fibre spinning.

# **Properties of Commerical Polymers**

12 Hrs

Polyethylune, polyvinyl chloride, polyamides, polyesters, phenolic resins, opoxy resins and silicone polymers. Functional polymers - Fire retarding polymers and electrically

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conducting polymers. Biomedical polymers -contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

# **Books Suggested**

- Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley. 1.
- 2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- 3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Ottanbrite.
- 4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- Physics and Chemistry of Polymers, J.M.G. Cowie, Blackle Academic and Professional. 5.

Paper VE(Research Aptitude in Chemistry)

UNIT 1: Foundation of Scientific Research: Definition & objectives of research, Motivation in Research, Scientific research, Inculcation of scientific temper, avoidance of prejudices and lax judgments, undue admiration of authority (i.e. excessive admiration of the work of great minds), false distinction between theoretical and applied research, various stages of scientific research, Importance of research, methodology in scientific research, research method vs research methodology, criteria of good research, quality of researcher, significance of research in Chemical sciences in Indian context.

UNIT 2: Research Methodology: Types of research, description vs. analytical, applied vs. fundamental, quantitative vs. qualitative, conceptual vs. empirical

UNIT 3: Research Formulation: Definition of research problem, necessity of defining research problem, criteria and characteristic of good research problem, hypothesis-meaning, types, importance of literature review in defining problem, selection of topic of research.

# UNIT 4: Literature of Chemistry and Survey

Print: Primary source Journal (Journal abbreviations and importance of ISSN No.), Papers, Notes, Communications (Letter), Patents of different fields of Chemistry (Organic Inorganic, Physical Polymer, Pharmaceuticals, Industrial and Analytical)

Secondary source- Listing of titles ,abstracts, Bielstein, compendia and tables of information, review, annual review, awareness service, general treatise, monograph and treaties on specific areas, understanding of terminology text, reference, comprehensive, survey, compendium hand desk, vocabulary regarding book.

Abstract: Type (Chemical, Physical, Analytical), survey of abstract indexes (substance index, author index, general technique index, collective and comprehensive indices).

Digital: Web resources, e-Journal access, TOC alerts, Hot articles, citation index, Impact factor, H-index, e- consortium, UGC infonet, e- books, internet discussion groups and communities blog, preprint server, search engines- Scirus, goole scholar, Chemindustry, Wiki-database, Chemspider, Science Direct, SciFinder, Scopus. Preparation of a review article related to the research problem of the student.

UNIT 5: Error Analysis: Various types of error, precision and accuracy, significant figure, various statistical test for accuracy results, positive and negative deviation from accuracy, the Gaussian distribution, The normal distribution of random error, mean value, variance and standard deviation, reliability intervals, deviation from the Gaussian law of error distribution, t-test, comparison of mean value with expected value, comparison of the result of the two different methods, comparison of the precision of two methods by F-test, Gross error, elimination of outlaying result, graphical methods, linear regression, regression line, standard deviation, correlation coefficient, multiple linear regression (one variable with two other variable).

UNIT 6: Fundamental Laboratory Techniques: Basic principles, health and safety, working with liquids, basic laboratory procedures, pH and buffer solutions.

UNIT 7: Report Writing: Types of report, writing scientific report, planning of writing, preparation, draft, revision, refining, research report format, writing literature surveys and reviews.

Types of scientific papers- Original research papers, review papers, symposium papers, invited papers, conference papers, and technical research papers.

Research report format - Title, abstract, introduction, materials and method, result, discussion, conclusions and references, acknowledgements, appendices. Research paper format in IJC, JICS, JACS, JCS, Tetrahedron, Analytical Chemistry, JCE, JHC etc.

#### Thesis:

Components – Titles, title page, dedication, preface, acknowledgements, table of contents, abstract, introduction, definition of the problem, prefatory notes, experimental section, result, discussion, conclusion, bibliography, references, appendices.

Special elements – Footnote, number, quantities, siunits, functions, mathematical expression and equations, tables, figure, captions, link between figure and text, line drawing, diagrams and graphs, half notes, punctuation, common proof marks that may be used to correct a manuscript.

UNIT 8: Financial Assistance: Role of funding agencies like UGC, CSIR, ICAR, ICMR, ISRO, DRDO, DST, DBT, CST in R&D of chemical sciences. Writing research proposal- Title and summary, justification, background, objectives, research plan and time schedule, dissemination of results, budget, collaborating institution, literature references, competence of applicants.

UNIT 9: Research Ethics: Plagiarism- Definition, consequences, avoidance

UNIT 10: Communication Information: Organizing a poster display, Giving oral presentation with help of effective slides, Knowledge about seminar, symposium, conferences, convention, congress, workshop.

#### Books:

- 1. Research Methodology, C.R. Kothari, New Age International Publication, 2004.
- 2. Practical Skills in Chemistry; Dean, Jones, Hollas, Reed, Weyers, Pearson Education Ltd.
- 3. Writing and Presentation Scientific Papers 2/e; Malmfors, Grossman, Viva Book Pvt, Ltd.
- 4. How to write a successful science Thesis; Russey, Ebel, Bliefest, Wiley-VCH.

# **Inorganic Chemistry Practical**

#### 1. Inorganic Preparation

- (i) NH<sub>4</sub>[Cr(SCN)<sub>4</sub>(NH<sub>3</sub>)<sub>2</sub>].H<sub>2</sub>O
- (ii) (NH<sub>4</sub>)<sub>2</sub> [PbCl<sub>6</sub>]
- (iii) Co[Hg(SCN)<sub>4</sub>]
- (iv) Ferric alum (ferric ammounium sulphate)
- (v) Prussian blue
- 2. Potentiometry
- a. Acid Base, redox and precipitation titration
- b. Determination of stability constants of suitable complex systems.
- 3. Conductometry
- 4. Calorimetry and Spectrophotometry

Estimation of the following metals in solution V, Cr, Mo, Fe and Ni

- 5. Flame Photometry
- a. Estimation of magnesium and calcium in tap water
- b. Estimation of calcium in calcium salt solution

#### 6. EDTA Titration

Estimation of Mg2+, Zn2+, and Mg2+ and Ca2+ in admixture

#### 7. Chromatography

- (i) Separation of Cl and Br by suitable ion exchangers
- (ii) Separation of Co2+ and Ni2+ by suitable ion exchangers
- (iii) Separation of Zn2+ and Mn2+ by suitable ion exchangers
- 8. Working out mass spectral fragmentation pattern and interpreting the molecular ion cluster peaks on the basis of El spectra of selected compounds.

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# System of Marking

Duration: 12h (2 days)	M.M: 75
Exercise 1: Inorganic Preparation (any one)	25
Exercise 2: Potentiometry/ Conductometry/ Colorimetry/ Spectrophotometry/ Flame Photometry/ EDTA titration	25
Exercise 3: Chromatographic separation / Interpretation of spectra	10
Viva- voce	10
Record	05

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#### **Organic Chemistry Practical**

#### 1. Qualitative analysis

Separation, purification and identification of components of ternary organic mixtures (liquid – liquid – liquid – liquid – solid – solid – solid – solid )

Each component should not contain more than two functional groups.

The student should check the purity by TLC.

Systematic analysis of each component leading to their final identification laying emphasis on solubility, element detection, melting point, boiling point determination, ignition test, unsaturation test, functional group test and preparation of suitable derivative.

### 2. Organic Synthesis: Multi-step synthesis

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

(i)	(Benzilic acid rea	arrangement)	Benzoin		Benzilic acid
(ii)	Nitrobenzenen		sym – '	Tribromoben	zene
(iii)	Aniline		p - Bro	moaniline	

#### 3. Chromatography

Separation and identification of the components present in the given organic mixture by chromatographic methods (Paper or TLC) and determination of Rf value

- (i) Sugars: glucose, fructose and sucrose
- (ii) Amino acids
- (iii) Fluorine, anthracene and diglyme (diethyl glucoxyldimethyl ether) (by TLC)
- (iv) Column chromatographic separation of pigments from green leaves

#### 4. Spectroscopy

Interpretation of Uv, IR, pmr, cmr, MS spectra of simple organic compounds Hydrocarbons, carbonyl compounds, hydroxyl compounds, amines, acids and their derivatives

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# System of Marking

Duration: 12h (2 days)	M.M: 100
Exercise 1: Organic mixture analysis	30
Exercise 2: Organic preparation (any one)	20
Exercise 3: Chromatographic separation or Interpretation of spectra	10
Viva- voce	10
Record	05
Tour / Seminar / Project work	2000 ·
	25

All type of spectra of a compound will be provided to student for structure elucidation on rotational basis.

Report of tour / seminar/ project work must be submitted in hard copy.

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# **Physical Chemistry Practical**

#### Section A

# Conductometry

- 1. Conductometric titration of a strong acid with a strong base
- 2. Conductometric titration of a strong acid with a weak base
- 3. Conductometric titration of a weak acid with a weak base
- 4. Conductometric titration of a mixture of a strong acid and a weak acid with a strong base
- 5. Conductometric titration of a weak acid with a strong base
- 6. To verify Ostwald's dilution law
- 7. To verify Kohlrausch's law

#### Section B

# pH - Metry

- 1. To titrate strong acid with a strong base pH metrically and calculate pKa value of an acid
- 2. To titrate strong acid with a weak base pH metrically
- 3. To titrate weak acid with a strong base pH metrically
- 4. To titrate mixture of a strong acid and a weak acid with a strong base pH metrically
- 5. To prepare a buffer solution and measure pH by pH meter
- 6. To verify Henderson equation

#### Section C

## Potentiometry

- 1. To titrate weak acid with strong base potentiometrically
- 2. To titrate strong acid with strong base potentiometrically
- 3. To titrate KCl, KBr and KI and mixture against AgNO<sub>3</sub> potentiometrically
- To estimate Fe(SO<sub>4</sub>). (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> solution potentiometrically and determine redox potential
- 5. To determine solubility of sparingly soluble salt potentiometrically

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# Optical

- 6. Colorimetry: To verify Lambert's Beer Law
- 7. Refractometer
- 8. Polarimetry

# Computational Experiments

- 1. Computer applications in Chemistry
- 2. Computer programming based on FORTAN77
- 3. Exposure to available standard packages like CHEMDRAW
- 4. Generation of graphs, data sheet creation and tables using EXCEL Programme
- 5. Geometry Optimization and energy calculation

# System of Marking

Duration: 12h (2 days)			M.M: 75
Exercise 1: Any one experiment from section A	×		20
Exercise 2: Any one experiment from section B	•		20
Exercise 3: Any one experiment from section C			_ 20
Viva- voce		Ø	10
Record			05

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