# M. Sc. Chemistry I to IV Semester

		Semes	ter I		
Code	Subject	Credit	Continuous Internal Assessment (CIA)	End Semester Exam. (ESE)	Total
M-Chem-101	Physical Chemistry I	5	30	70	100
M-Chem-102	Inorganic Chemistry I	5	30	70	100
M-Chem-103	Organic Chemistry I	5	30	70	100
M-Chem-104 Phys	Physical & Inorganic Chemistry Practical I	5	30	70	100
		20	120	280	400

		Semeste	r II		
Code	Subject	Credit	Continuous Internal Assessment (CIA)	End Semester Exam. (ESE)	Total
M-Chem-201	Physical Chemistry II	5	30	70	100
M-Chem-202	Inorganic Chemistry II	5	30	70	100
M-Chem-203	Organic Chemistry II	5	30	70	100
M-Chem-204	Physical & Inorganic Chemistry Practical II	5	30	70	100
	Citemony - Identity	20	120	280	400

		Semest	er III		
Code	Subject	Credit	Continuous Internal Assessment (CIA)	End Semester Exam. (ESE)	Total
M-Chem-301	Physical Chemistry III	5	30	70	100
M-Chem-302	Inorganic Chemistry III	5	30	70	100
M-Chem-303	Organic Chemistry III	5	30	70	100
M-Chem-304	Organic Chemistry Practical III	5	30	70	100
	Truction III	20	120	280	400

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		Semest	er IV		
Code	Subject	Credit	Continuous Internal Assessment (CIA)	End Semester Exam. (ESE)	Total
M-Chem-401	Elective Physical Chemistry I-IV	5	30	70	100
M-Chem-402	Elective Inorganic Chemistry I-IV	5	30	70	100
M-Chem-403	Elective Organic Chemistry I-IV	5	30	70	100
M-Chem-404	Elective Physical, Inorganic & Organic Chemistry Practical	5	30	70	100
	F	20	120	280	400

Code	Subject	Credit	Continuous Internal Assessment (CIA)	End Semester Exam. (ESE)	Total
	Physical (	Chemistry	Elective Papers		
M-Chem-401 (A)	Advance Statistical Thermodyanamics	5	30	70	100
M-Chem-402 (A)	Advance Chemical Reaction Dyanamics	5	30	70	100
M-Chem-403 . (A)	Advance Quantum Chemistry	5	30	70	100
M-Chem-404 (A)	Physical Practical	5	30	70	100
	Inorganic	Chemistr	y Elective Papers		
M-Chem-401 (B)	Ligand Field Theory	5	30	70	100
M-Chem-402 (B)	Reaction Mechanism and Supramolecular Chemistry	5	30	70	100
M-Chem-403 (B)	Organotransition Metal Chemistry and Metal clusters	5	30	70	100
M-Chem-404 (B)	Inorganica Practical	5	30	70	100
	Organic (	Chemistry	Elective Papers		
M-Chem-401 (C)	Organic Synthesis	5	30	70	100
M-Chem-402 (C)	Chemistry of Natural Products	5	30	70	100
M-Chem-403 (C)	Medicinal Heterocyclic Chemistry	5	30	70	100
M-Chem-404 (C)	Organic Practical	5	30	70	100

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M.Sc.(Chemistry) Semester-I M-Chem -101 Physical Chemistry

Full Marks: 70 Time - 3 Hours Part-A 10 x 2=20 Marks Ten Multiple Choice Questions (Compulsory) (Two Questions from each unit) Part-B 4 x 5=20 Marks Five Short Answer Question (Four to be Answered) (One Question from each unit) Part-C

10 x 3=30 Marks Three Long Answer Question (Three to be Answered) (One Question from each unit)

# Unit I: Classical Thermodynamics and Statistical Thermodynamics

Classical Thermodynamics: Brief review of concepts of laws of thermodynamics, free energy, chemical potential and entropy, Concept of partial molar properties and their significance-partial molar free energy, partial molar volume, partial molar heat content, Determination of these quantities, Gibbs-Duhem equation, Concept of fugacity, Determination of fugacity by graphical method and compressibility factor method, Thermodynamics of Ideal and Non-Ideal solutions. Determination of Excess thermodynamic function, GE, SE, HE etc, Activity and activity coefficient: Determination of activity coefficient by EMF and solubility method.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of "distributions". Thermodynamic probability, Most probable distribution, Statistical Mechanics for systems of independent particles and its importance in chemistry, Types of statistics-Maxwell-Botzmann, Bose-Einstein and Fermi-Dirac statistics, Derivation of distribution laws for the three types of statistics, Concept of Microstates and Macro states, Partition Function (Definition and significance): Translational, rotational, vibrational and electronic partition functions, Molecular partition functions, Relation between thermodynamic functions (U, H,S,G and C<sub>v</sub>) and the partition functions. Applications of partition functions, Lagrange's undetermined multipliers, Stirling's approximation, Heat capacity, behavior of solids - chemical equilibrium constant in terms of partition functions.

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#### Unit II: Chemical Kinetics

Chemical kinetics, rate of reactions, factors influencing the rate of reaction. Kinetics of side reaction, opposing reaction and consecutive reactions, Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenius equation-characteristics, significance of activation energy, effect of temperature on rate of reaction.

Concept of Steady state kinetics, Chain reactions. Photochemical reactions between hydrogen and bromine, hydrogen and chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Mechanism and kinetics of pyrolysis of acetaldehyde, decomposition of ethane and photo dimerisation of anthracene.

### Unit III: Electrochemistry

Electrochemistry of solutions: Activity coefficients and ion-ion interactions, Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination, Ionic strength, Derivation of Debye-Huckel theory for the problem of activity coefficients, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-Huckel-Onsagar conductance equation and its extension to ion solvent interactions.

Overpotential, exchange current density, Derivation of Butler-Volmer equation, Tafel Plot. Electrocatalysis: Definition and Influence of various parameters. Polarography, Ilkovic equation, half wave potential and its significance.

# Unit IV: Solid State Chemistry and Surface Chemistry

#### Solid State Chemistry

X-ray diffraction by crystals, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scattering factor and structure factor, intensities from atomic positions for BCC and FCC lattices, Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier transform of the structure factor.

# **Surface Chemistry**

Surface tension, capillary action, Review of adsorption curves, Adsorption-desorption, Adsorption forces, Heat of adsorption- Types, Measurements of heat of adsorption (Calorimetric and Clausius-Clapeyron method), Measurement of adsorption isotherms, (Volumetric and Gravimetric methods), Determination of entropy of adsorption, Electrostatic adsorption, adsorption indicators and their applications. Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles.

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# Unit V: Quantum Chemistry

Introduction to quantum mechanics, Postulates of quantum mechanics, Schrödinger wave equation, Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian operators, Commutation of operators, Normalization and orthogonality of wave functions, Average (expectation) values, Heisenberg's Uncertainty principle, Eigenfunctions and Eigenvalues. Physical Interpretation of wave function.

Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three dimensional box, Quantum mechanical degeneracy, tunneling (no derivation), Application of Schrödinger equation to harmonic oscillator, rigid rotator, Solution of  $R, \Theta, \Phi$ , equation, Angular Momentum operators and their properties, Eigen functions and Eigen values of angular momentum, Ladder operator method for angular momentum.

Hydrogen atom in spherical polar co-ordinates, Total wave function of hydrogen atom, Quantum numbers and their characteristics, List of wave functions for few initial states of hydrogen like atoms, Diagrams of radial and angular wave functions, Radial and angular distribution function and their significance, Electron spin (Stern-Gerlach experiment), spin-orbital, symmetry and anti-symmetry and Pauli-exclusion principle.

# SUGGESTED BOOKS:

- Molecular thermodynamics by Donald A. Mc Quarrie. John D. Simon University Science Books California.
- 2. Thermodynamics by Rajaraman and Kuriacose. East-West Press.
- 3. Statistical Thermodynamics by M. C. Gupta. Wiley Eastern Ltd.
- 4. Elements of Statistical Thermodynamics by Leonard K. Nash (Courier Corporation).
- 5. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley.
- 6. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid. Pearson Education inc.
- Modern Electrochemistry Vol-1 and II by J. O. M Bockris and A. K. N. Reddy. Plenum New York.
- 8. Electrochemistry, Principles and applications by Edmund, C. Potter. Cleaver-Hume Press London.

9. Principles and applications of Electrochemistry by D. R. Crow, Chapman and Hall, London.

10. Solid State Chemistry by A.R. West, John Wiley, N.Y.

11. Quantum Chemistry by D.A. McQuarrie Viva. New Delhi.

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M.Sc. (Chemistry)
Semester-I
M-Chem -102
Inorganic Chemistry

Part-A

Ten Multiple Choice Questions (Compulsory) 10 x 2=20 Marks

(Two Questions from each unit)

Part-B

Five Short Answer Question (Four to be Answered) 4 x 5=20 Marks

(One Question from each unit)

Part-C

Three Long Answer Question (Three to be Answered)

10 x 3=30 Marks

(One Question from each unit)

# Unit I: Stereochemistry and Bonding of compounds of main group

VSEPR model, shapes of molecules-ClF<sub>3</sub>, ICl<sub>4</sub>, TeF<sub>5</sub>, I<sub>3</sub>, TeCl<sub>6</sub><sup>2</sup>, XeF<sub>6</sub>, SbCl<sub>6</sub><sup>3</sup>, IF<sub>7</sub>, ReF<sub>7</sub>, XeF<sub>8</sub><sup>2</sup>, TaF<sub>8</sub><sup>3</sup>, Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding, Some simple reactions of covalently bonded molecules, electron deficiency and structural aspects of boranes, carboranes, Wade's rule, Metal – Metal multiple bonding. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic (CO, NO, HF, ICl) and triatomic molecules (CO<sub>2</sub> and NO<sub>2</sub>).

### Unit II: Nuclear Chemistry

Shell Model, liquid drop model, Nuclear reactions and their types, Nuclear reaction cross – section, Fermi gas model, Collective model and Optical model. Detection and measurement of radiation, G.M. and Scintillation counters, Nuclear reactors. Application of radio isotopes, Tracer technique, neutron activation analysis, isotopic dilution method, radiation hazards.

# Unit III: Chemistry of Lanthanides and Actinides

Position in the periodic table, oxidation states and their stability, Lanthanide and Actinide contraction, Magnetic and Spectral properties, Separation technique (Ion exchange and Solvent extraction). Transuranic elements, Synthesis and Chemistry of Np and Pu, Separation of Pu from Spent fuel. The minerals of lanthanides and actinides and their occurrence in India.

# Unit IV: Group theory and its applications

Classification of molecules into point groups. Defining properties of a mathematical group, Symmetry operation of a molecule as elements of a mathematical group, subgroups, concept of conjugate and class, similarity transformation.

# Unit V: Matrix representations for symmetry operations

Reducible and Irreducible representations Character. The Great orthogonality theorem (derivation not required). Consequences of orthogonality theorem, character table, construction of Character table for  $C_{2v}$  and  $C_{3v}$ . Direct product, reduction formula. Wave functions as bases of irreducible representations (p – and d- orbitals),

Symmetry: Intrared and Raman's spectroscopy. SALCs, Projection operators, Illustrative examples. Hybridisation and its application, M.O. using group theory

#### SUGGESTED BOOKS:

- 1. Chemical Application of group Theoryby Cotton, F.A. Wiley Interscience: N.Y.
- 2. Chemical Group Theory and symmetry in chemistry by Gurdeep Raj, Ajay Bhagi& Vinod Jain.
- 3. Elements of Nuclear Chemistry by H. JArnikar. Wiley Eastern Ltd.
- 4. The chemistry of the Actinides elements by Joseph J. Katz & G.T. seaberg.
- 5. Problems in structural Chemistry by Hatfield W.F & Palmer, R.A.W.A Benjamin, Inc. N.Y.

6. Textbook of inorganic chemistry by Sodhi, G. S. Viva books Pvt. Ltd.

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M.Sc. (Chemistry)
Semester-I
M-Chem -103
Organic Chemistry

Time - 3 Hours Full Marks: 70

Part-A

Ten Multiple Choice Questions (Compulsory) 10 x 2=20 Marks

(Two Questions from each unit)

Part-B

Five Short Answer Question (Four to be Answered) 4 x 5=20 Marks

(One Question from each unit)

Part-C

Three Long Answer Question (Three to be Answered)

10x 3=30 Marks

(One Question from each unit)

#### Unit I:

(a) Nature of Bonding in organic Molecules: Delocalized Chemical Bonding – conjugation, cross conjugation, resonance, hyper- conjugation, tautomerism. Bonding in fullerenes. Aromaticity in benzenoid and non – benzenoid compounds, Huckel's rule, energy level of molecular orbitals; anti – aromaticity, PMO theory and its applications. Chemistry of tropones, tropolones, azulenes, metallocenes and annulenes. Bonding in addition compounds, crown ether complexes, inclusion compounds, cyclodextrins and catenanes.

#### (b) Aromatic substitution:

- i) Aromatic electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho / para ratio, ipso attack, orientation in other ring systems.
- ii) Aromatic nucleophilic Substitution: The S<sub>N</sub>Ar, S<sub>N</sub>1 and benzyne mechanism. Reactivity: effect of substrate structure, leaving group and attacking nucleophile.

#### Unit II:

Stereochemistry: Chirality, molecules with more than one chiral center, threo and erythro isomers, specific rotation, racemisation, methods of resolution, enantiotopic and diastereotopic atoms & groups, stereospecific and stereoselective synthesis, asymmetric synthesis.

Axial chirality: optical activity of biphenyls, allens, alkylidene cycloalkanes and spiranes, Planar chirality: optical activity of ansa compound and cyclophanes. Chirality due to helical shape. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. Conformation due to rotation about C-C single bond in acyclic molecules. Conformation of

cyclohexanes (monosubstituted and disubstituted) and decalins, effect of conformation on reactivity of acyclic and cyclic molecules.

#### Unit III:

Reaction Mechanism: Structure and Reactivity: Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin – Hammett principle, Potential energy diagram, Transition states and reaction intermediates, methods of determining mechanisms, isotope effect, Hard and soft acids and bases. Generation, structure, stability and reactivity of free radicals carbenes and nitrenes. Hammett equation and linear free energy relationship, substituent and reaction constants.

#### Unit IV:

- (a) Addition to C=C and  $C \equiv C$  bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophile, nucleophile and free radicals, regio selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, Oxymercuration demercuration, Hydroboration-oxidation, Iodolactonization, Prevost reactions (dry and wet methods). Addition of carbenes, Simmons- Smith reaction, Epoxidation, sharpless asymmetric expoxidation. Michael Addition.
- (b) Addition to C= O bond: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters. Wittig reaction. Wadsworth-Emmons reaction. Aldol condensation, Knoevengel reaction, Claisen reaction, Mannich reaction, Benzoin condensation, Perkin reaction and Stobbe reaction. Robinson annulations reaction. Cram's rules of diastereo selection. Stork enmine synthesis, concept and application of Umpolung use of propane-1, 3-dithiol. Sulphurylides.
- (c) Elimination reactions: The E1, E2 and E1CB mechanisms and stereochemistry of these reactions in acyclic and cyclic molecules. Effect of substrate structure, strength of the bases used, leaving groups and the reaction medium on E1, E2 and E1CB reactions. Mechanism and orientation in pyrolytic eliminations (E<sub>i</sub> reactions) of: Esters of carboxylic acid, methyl xanthate(Chugaev reaction), tertiary amine oxides(Cope elimination), Sulphoxides and selenoxides. Shapiro reaction and Peterson's reaction for synthesis of alkanes.
- d) Aliphatic nucleophilic Substitution:  $S_N1$ ,  $S_N2$  and  $S_Ni$  reactions, their mechanism and Steriochemistry. Distintion between  $S_N1$  and  $S_N2$  reaction by isotopic labeling. Nucleophilicity versus basicity. Neighboring group participation: stereochemistry and anchimeric assistance. Nucleophilic acyl substitution: Hydrolysis of esters of carboxylic acid  $B_{AC}2$  and  $A_{AC}2$  mechanisms.

# Unit V:

Free radical reactions: Free radical substitution mechanism, mechanism at an aliphatic and aromatic substrates and at bridgehead. The effect of solvent on reactivity. Allylic halogenation. Oxidation of aldehydes to carboxylic acids. Coupling of alkynes and arylation

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of aromatic compounds and active alkenes by diazonium salts, Sandmeyer reaction, Hunsdiecker reaction, Suzuki reaction.

# SUGGESTED BOOKS:

- Advanced Organic Chemistry: Reactions, Mechanism and Structure by Jery March. John Wiley.
- 2. Advanced Organic Chemistry (Parts A & B) by F.A. Carey and R.J. Sundberg, Plenum Press.
- 3. Stereochemistry of Organic Compounds by D. Nasipuri. New Age International.
- 4. Reaction Mechanism in Organic Chemistry by S.M. Mukherji and S.P. Singh. Macmillian.
- 5. Principles of Organic Synthesis by R.O.C Norman and J.M. Coxon, Blackie Academic & Professional.

6. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley Eastern Ltd., New Delhi.

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# M. Sc. (Chemistry) Semester-I M-Chem-104

# Physical Lab Course (General)

Time – 6 Hours Full Marks: 70

- 1. Water equivalent of calorimeter and determination of
  - i. Heat of solution of potassium nitrate.
  - ii. Heat of neutralization of strong acid and strong base.
  - iii. Heat of solution of oxalic acid from solubility measurement.
  - iv. Basicity of polybasic acids.
- 2. Molecular weight of a non-electrolyte by Ebullioscopic method.
- 3. Molecular weight of a non-electrolyte by cryoscopic method.
- 4. Saponification of ethyl acetate with sodium hydroxide by chemical method.
- 5. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
- 6. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
- 7. Distribution coefficient of-
  - (a) Acetic acid
  - (b) Benzoic acid between water and Benzene by partition method.
- 8. Determination of specific and molecular rotation of sucrose in different concentrations and to determine the concentration of given solution.
- 9. Rate constant of acid catalyzed hydrolysis of sucrose/Cane suger by polarimetric method.
- 10. Conductometric Experiments:

Determination of-

- i. Dissociation constant of acetic acid.
- ii. Equivalence point between acid-base titration of NaOH with HCl solutions.
- iii. Equivalence point between a mixture of HCl and CH<sub>3</sub>COOH with NaOH.
- iv. Solubility product (K<sub>sp</sub>) of sparingly soluble salt, e.g. AgCl, BaSO<sub>4</sub>
- 11. Potentiometric Experiments-

Determination of-

- i. EMF of concentration cell
- ii. pH of a given solution using hydrogen electrode and quinhydrone electrode
- iii. Equivalence point in Acid-Base titration
- iv. Equivalence point in precipitation titration (AgNO<sub>3</sub>vrsNaCl).
- 12. Determination of pH of a Buffer solutions
- 13. Preparation of colloidal solution of

i. As<sub>2</sub>S<sub>3</sub> Sol.

ii. Fe(OH)3 Sql

50 Marks

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14. Viva-Voce

10 Marks

15. Record of Practical Note Book

10 Marks

#### SUGGETED BOOKS:

- 1. Findlays practical physical chemistry revised by P. B. Levitt, Longman's London.
- 2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed.
- 3. Practical Physical Chemistry by B. Viswanathan& P.S. Raghwan, Viva Books Pvt. Ltd., New Delhi.
- 4. Experiments in Physical chemistry by J.C. Ghosh, Bharti Bhawan, Patna.
- 5. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut.
- 6. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi.
- 7. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York.
- 8. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd
- 9. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York.
- 10. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi.
- 11. Experimental Physical Chemistry by V. D. Atavale and ParulMathur, New Age International, New York.
- 12. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co. new York.

13. Practical's in physical chemistry: A. Modern Approach by P.S Sindhu, Mac. Milian Publishers Delhi (2006).

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# M. Sc. (Chemistry) Semester-I M-Chem-104 Inorganic Lab course (General)

Time - 6 Hours

Full Marks: 70

- Micro and Semi micro qualitative analysis of mixtures containing two anions, two common cations and one less familiar elements: Cr, Mo, W, V and Mn
- 2. Qualitative analysis: To analyse quantitatively two constituent ions of the following estimated using EDTA.:
  - (a) Cu, Zn
  - (b) Ni, Fe
  - (c) Ca, Mg
  - (d) Al, Mg.
- 3. Inorganic Preparations
  - (a) Pot. trioxalatoferrate (III)
  - (b) Pot. trioxalatochromate (III)
  - (c) Diaquodioxalatochromate (III)
  - (d) Hexaminenickel (II) chloride

50 Marks

4. Viva-Voce 10 Marks

5. Record of Practical Note Book

10 Marks

## SUGGESTED BOOKS:

- Vogel's Text book of Qualitative Chemical Analysis by J. Bassett, G. H. Jeffery and J. Mendham, ELBS.
- 2. Vogel's text book of Quantitative Chemical Analysis, 5<sup>th</sup> Edition by J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical.
- 3. Inorganic Semimicro Qualitative Analysis by V. V. Ramanujam; The National Pub. Co.

4. Practical Inorganic Chemistry by G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London.

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M.Sc. (Chemistry)
Semester-II
M-Chem-201
Physical Chemistry

Time: 3 Hours Full Marks: 70

Part-A

Ten Multiple Choice Questions (Compulsory) 10 x 2=20 Marks

(Two Questions from each unit)

Part-B

Five Short Answer Question (Four to be Answered) 4 x 5=20 Marks

(One Question from each unit)

Part-C

Three Long Answer Question (Three to be Answered)

10 x 3=30 Marks

(One Question from each unit)

# Unit I: Quantum Chemistry - Approximate methods and Chemical Bonding

Approximate methods: The Variation theorem; linear variation principle; Perturbation theory (first order and non-degenerate); Applications of variation method and perturbation theory to Helium atom. Chemical Bonding: Born-Oppenheimer approximation; Valence bond (VB) and Molecular orbital (LCAO) treatment (MO) of hydrogen atom; Comparison of MO and VB treatments; Configuration interactions; Extension of MO treatment to homo nuclear and hetero nuclear systems; Hückel Molecular Orbital Theory/Method (HMO), Application to  $\pi$  system-ethylene, Allyl system, Butadiene, Cyclopentadienyl & benzene system. Calculation of properties-delocalization energy, electron density bond order, free valence; Introduction to Extended Hückel Theory.

# Unit II: Electronic Properties and Band Theory

Electronic structure of solids- band theory, Refinement to simple band theory; Band structure of metals, insulators and semi conductors; Intrinsic and extrinsic semiconductors; Doped semi conductors; p-n junctions; Light Emitting Diode (LED): Principle and applications, Blue LED, Nanoscope.

# Unit III: Superconductors

High-T<sub>c</sub> Oxide Superconductors: Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure; Normal state properties: anisotropy and temperature dependence of electrical resistance; Superconducting state: heat capacity, coherence length, relation between

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 $T_c$  and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high  $T_c$ -cuprates. Ceramics composites and nanomaterials.

Organic Materials: Conducting organics-Metals from molecules, charge transfer materials and conducting polymers; Organic superconductors; Fullerenes. Molecular ferromagnets and ferroelectrics; Liquid crystals: mesomorphic behavior, optical properties of liquid crystals, display devices.

# Unit IV: Conducting Polymers and Solid State Chemistry

**Electrical conducting polymer:** Conducting polymers-Polyacetylene (PA), Polyparaphenylene (PPP), Polyaniline (PANI), Polyphenylene sulfide (PPS), Polypyrrole (PPY)-mechanism of conduction and applications.

Solid State Chemistry: Perfect and Imperfect crystals, intrinsic and extrinsic defects point defects, line and plane defects, vacancies-Schotty defects and Frenkel defects. Thermodynamics of Schotty and Frenkel defect formation, colour centers, non-stoichiometry defects.

# Unit V: Electrochemistry-Corrosion and Cyclic Voltammetry

Corrosion: Scope and economics of corrosion, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), units of corrosion rate, passivity and its breakdown, Corrosion prevention (electrochemical, inhibitor and coating methods).

Cyclic Voltammetry: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry, interpretation of voltammograms.

# SUGGESTED BOOKS:

- 1. Physical Chemistry by P. Atkins and J. D. Paula, 9th Ed., Oxford University Press.
- 2. Quantum Chemistry by D.A. McQuarrie Viva, New Delhi.
- 3. Quantum Chemistry by J.P. Lowe & K. Peterson, Academic Press.
- 4. Elementary Quantum Chemistry by F.L., Pilar, Dover Publication, N.Y.
- 5. Principles of Quantum Chemistry by Ram Yatan Prasad, Foundation Books, New Delhi 2015.
- 6. Introduction to Quantum Chemistry by A. K. Chandra, Tata McGraw Hill.
- 7. Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey.
- 8. Quantum Chemistry by R. K. Prasad, New Age International.
- 9. Quantum Chemistry through problems and solutions by R. K. Prasad, New Age International.
- 10. Introduction to Solids by L.V. Azaroff, Tata McGraw-Hill, New Delhi.

- 11. Solid State Chemistry by A.R. West, John Wiley, N.Y.
- 12. New Directions in Solid State Chemistry by C.N R. Rao and J. Gopalkrishnan, Cambridge Univ. Press.
- 13. Superconductivity Today by T. V. Ramakrishnan and C.N.R. Rao, Wiley Eastern Ltd., New Delhi.
- 14. Designing the Molecular World: Chemistry at the Frontier by P. Ball, Princeton Univ. Press.
- 15. An Introduction to Solid State chemistry by E. More and L. Smart, Chapman & Hall.
- 16. Crystal Structure Determination by W. Massa, Springer.
- 17. Principles of Solid State by H.V. Kerr, Wiley Eastern Ltd.
- 18. Text book of Polymer science by F.W. Billimeyer, Wiley-Interscience, N.Y.
- 19. Introduction to polymers by R.J. Young & P.A. Lovell, Chapman and Hall.
- 20. Modern Electrochemistry (Vol.1,,2A and 2B) by Bockris and Reddy, Plenum, N.Y.
- 21. Polarography and Allied Techniques by V SuryanarayanaRao, Universities Press (India) Pvt. Ltd., Hyderadad.
- 22. Basic concepts of Analytical Chemistry by S M Khopkar, New Age International Publishers, third edition, New Delhi, 2008.
- 23. Electrochemical Methods- Fundamentals and Applications, 2<sup>nd</sup>Ed. by A J Bard and L R Faulkner, John Wiley & Sons Inc., New York.
- 24. Chemical and Electrochemical Energy systems by Narayan and Viswanathan, Hyderabad, Universities Press (India) Pvt. Ltd., Hyderadad.
- 25. Understanding Batteries, RM Dell and DAJ Rand, Fuel cells and their applications by Karl kordesh, gunter, Simader, VCH-Weinheim, Cambridge.
- 26. Fundamentals of electrochemical deposition by Milan Paunovic and Mordechay Schlesinger, Wiley-interscience publications, New York.
- 27. Electrodeposition and Corrosion Control by J. M. West, J. Wiley W. Reviseded. Corrosion Handbook, Electrochemical Society Series, John Wiley and Sons.
- 28. Electrochemistry and corrosion science by Nestor Perez, Springer (India) Pvt. Ltd.
- 29. Principles and Prevention of Corrosion by D. A. Jones, Macmillan Publ. Co.
- 30. Bioelectrochemistry: Fundamentals, experimental techniques and application by P. N. Bartlett, Wiley& Sons.

31. Synthetic organic Electrochemistry by A M Fry, 2<sup>nd</sup> ed., Wiley.

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# M.Sc. (Chemistry) Semester-II M-Chem-202 Coordination chemistry

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	^	10 x 3=30 Marks

# Unit I: Magnetic Behavior of Substances

(One Question from each unit)

The orbital and spin effects on paramagnetism. Derivation of Russel /Saunder's terms, spin orbit interaction, Magnetic moment for large and small multiplet width, Quenching of orbital contribution, Magnetic properties of complex compounds.

# Unit II: Bonding in Coordination Compounds

Crystal Field theory, d- orbital splitting in cubic and non- cubic fields. Measurement of 10 Dq and factors affecting it. Splitting of S, P, D and F terms in Octahedral and Tetrahedral Symmetry, Limitation of C.F.T.

Evidences in support of covalent bonding in Transition metal complexes, M.O. Theory for  $ML_6n^+$  with  $\sigma$  and  $\pi$  bonding ligands using symmetry arguments, Magnetic properties and charge transfer spectra on the basis of M.O. model.

# Unit III: Spectral, Structural and Thermodynamic aspects of Crystal Field theory

Electronic Spectra: Selection rules for d-d transitions, and its breakdown .Electronic Spectra of d<sup>1</sup>,d<sup>2</sup>,d<sup>8</sup>and d<sup>9</sup> systems. Spectro chemical series. Crystal field effect on ionic radii of 3d ions, Jahn Teller distortion, Thermodynamic effects, Lattice energy and Hydration energy of octahedral complexes of 3d series, Site selection in normal and inverse spinel structure. Stepwise and overall stability constants, Determination of stability constant by Bjerrum and emf methods, Job's continuous variation method.

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# Unit IV: Substitution reaction in Transition Metal Complexes

Nature of substitution reaction. Lability and inertness of complexes, D, A, Id and Ia mechanisms, Substitution reaction in octahedral Co (III)complexes. Acid and base hydrolysis  $S_N^1CB$  hydrolysis, factors governing the rate of reaction, substitution without cleavage of metal – ligand bond. Mechanism of substitution reaction of Square planar complexes of Pt (II). Trans effect, Theories of trans effect.

### Unit V: Metal Carbonyls and Nitrosyls

Mononuclear and polynuclear carbonyls and their structures. Nature of M-C –O bonding. Preparation of metal carbonyls and their reactions, vibrational spectra of metal carbonyls.

Metal nitrosyls – bonding and structure. Metal carbonyl – nitrosyl complexes. Metal carbonyl hydrides.

### SUGGESTED BOOKS:

- 1. Elements of Magneto chemistry by R.L. Dutta & A. Syamal, Affilated East West Press Pvt. Ltd. New Delhi.
- 2. Concept and Model of Inorganic chemistry by BodieDouglus, Drl Mc Daniel, John Alexander, John Wiley & Sons Inc. New York
- 3. Inorganic Chemistry, Principles and structures and reactivity by James E. Huheey& Ellen A. Ketter, Pearson Education Asia.
- Concise Co-ordination chemistry by R. Gopalan & V. Ramalingam, Vikas Publication House.
- 5. Selected Topic in Inorganic Chemistry by Mallick, Madan & Tuli.
- 6. Mechanism of Inorganic Reactions by F. Basalo and R. G. Pearson, Wiley Eastern Ltd., New Delhi.
- 7. Inorganic Chemistry by D. F. Shriver and P. W. Atkins, ELBS, London.
- 8. Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson, John Wiley & Sons, New York.
- Electronic Absorption Spectroscopy and Related Techniques by D.N. Sathyanarayana, Universities Press (India) Ltd., Hyderabad.

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# M.Sc. (Chemistry) Semester-II M-Chem- 203 Chemistry of Biomolecules

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C	~	
Three Long Answer Question (Three to be Answered)		10 x 3=30 Marks
(One Question from each unit)		

# Unit I: Carbohydrate

Open chain and cyclic structure of monosaccharides: Configurations and conformation of monosaccharides, structure and functions of important derivatives of monosaccharides – glycosides, deoxysugars, aminosugars, N – acetylmuramic acids. Disaccharides – structure determination and chemical synthesis (Sucrose, Lactose, Maltose and Cellobiose). Polysaccharides -structural (Cellulose and Chitin), storage (Starch and Glycogen). Structure of glucosaminoglycons, carbohydrates of glycolipids.

## Unit II: Amino Acids and Peptides and Lipids

(a) Amino Acids, Peptides and Proteins: Definition, classification, stereochemistry, acid base properties, reactions and synthesis of amino acids. Isoelectric point of amino acid and peptides. Structure of peptide bonds. Amino acid sequencing. Chemical and enzymatic hydrolysis of proteins, Secondary structure of proteins, forces responsible for secondary structure of proteins,  $\alpha$ -helix,  $\beta$ -sheet, super secondary structure, tertiary structure of proteins – folding and domain structure and quaternary structure.

(b) Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerols. Glycophospholipids, lipoproteins, biological membranes, lipid metabolism,  $\beta$  – oxidation of fatty acids.

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#### Unit III: Nucleotides and Nucleic acids

Chemical properties and synthesis of pyrimidine and purine derivatives. Purine and pyrimidine bases in nucleic acids. Base pairing via H-bonding. Structure of Ribonucleic acid (RNA) and Deoxyribonucleic acid (DNA). Double helical model of DNA. Chemical and enzymatic hydrolysis of nucleic acids. An overview of gene expression : replication, transcription and translation. Genetic code.

# Unit IV: Terpenoids

Introduction, classification, Isoprene rule, Elucidation of structure determination and synthesis of the following compounds – Citral, α-Terpineol, Linalool and Camphor.

#### Unit V: Alkaloids

Introduction, classification, general methods of structure determination. Structure determination and synthesis of the following compounds - Nicotine, Papaverine and Atropine.

#### SUGGESTED BOOKS:

- 1. Concise Text Book of Biochemistry by T. N. Pattabhiraman, All India Publishers.
- 2. Biochemistry by A. L. Lehninger et. al., CBS.
- 3. A Text Book of Biochemistry by A. V. S. S. Rama Rao, UBSPD.
- 4. Biochemistry by P. C. Champe and R. A. Harvey, J. B. Lipincott& Co.
- 5. Fundamentals of Biochemistry by J. L. Jain, S. Chand & Co.
- 6. Biochemistry by COSIP-ULP, Bangalore University.
- 7. Outlines of Biochemistry by Conn E. E and StumpfP. K., John Wiley & Sons.
- 8. General Biochemistry by Weil J. H., Wiley Eastern
- 9. Biochemistry by Campbell M. K., Harcourt Brace & Co.
- 10. Principles of Biochemistry by Voet& Pratt.
- 11. Illustrated Reviews of Biochemistry by Harper.

12. Biochemistry by Stryer.

# M. Sc. (Chemistry) Semester-II M-Chem-204 Physical Lab Course

#### Time - 6 Hours

Full Marks: 70

- 1. Water equivalent of calorimeter and determination of
  - i. Heat of solution of potassium nitrate.
  - ii. Heat of neutralization of strong acid and strong base.
  - iii. Heat of solution of oxalic acid from solubility measurement.
  - iv. Basicity of polybasic acids.
- 2. Molecular weight of a non-electrolyte by Ebullioscopic method.
- 3. Molecular weight of a non-electrolyte by cryoscopic method.
- 4. Saponification of ethyl acetate with sodium hydroxide by chemical method.
- 5. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
- 6. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
- 7. Distribution coefficient of-
  - (a) Acetic acid
  - (b) Benzoic acid between water and Benzene by partition method.
- 8. Determination of specific and molecular rotation of sucrose in different concentrations and to determine the concentration of given solution.
- 9. Rate constant of acid catalyzed hydrolysis of sucrose/Cane suger by polarimetric method.
- 10. Conductometric Experiments:

Determination of-

- i. Dissociation constant of acetic acid.
- ii. Equivalence point between acid-base titration of NaOH with HCl solutions.
- iii. Equivalence point between a mixture of HCl and CH<sub>3</sub>COOH with NaOH.
- iv. Solubility product (Ksp) of sparingly soluble salt, e.g. AgCl, BaSO4
- 11. Potentiometric Experiments:

Determination of-

- i. EMF of concentration cell
- ii. pH of a given solution using hydrogen electrode and quinhydrone electrode
- iii. Equivalence point in Acid-Base titration
- iv. Equivalence point in precipitation titration (AgNO<sub>3</sub> vs NaCl).

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- 12. Determination of pH of aBuffer solutions
- 13. Preparation of colloidal solution of
  - i. As<sub>2</sub>S<sub>3</sub> Sol.
  - ii. Fe(OH)3 Sol.

50 Marks

14. Viva-Voce

10 Marks

15. Record of Practical Note Book

10 Marks

#### SUGGETED BOOKS:

- 1. Findlays Practical Physical Chemistry (revised) by P. B. Levitt, Longman's London.
- 2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed.
- 3. Practical Physical Chemistry by B. Viswanathan & P.S. Raghwan: Viva Books Pvt. Ltd., New Delhi.
- 4. Experiments in Physical Chemistry by J.C. Ghosh, Bharti Bhawan, Patna.
- 5. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut.
- 6. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi.
- 7. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York.
- 8. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd.
- 9. Experimental Physical Chemistry by Wilson, Newcombe& others, Pergamon Press, New York.
- 10. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi.
- 11. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York.
- 12. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co.new York.

13. Practical's in Physical Chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi.

# M.Sc. (Chemistry) Semester-II M-Chem-204 Inorganic Lab course

Time – 6 Hours Full Marks: 70

- 1. Micro and Semi micro qualitative analysis of mixtures containing two anions, two Common cations and one less familiar elements: Cr, Mo, W, V and Mn.
- 2. Qualitative analysis

To analyse quantitatively two constituent ions of the following estimated using EDTA:

- (a) Cu, Zn
- (b) Ni, Fe
- (c) Ca, Mg
- (d) Al, Mg. The cataions Mg<sup>2+</sup>,Ca<sup>2+</sup>ans Al<sup>3+</sup>.
- 3. Inorganic Preparations
  - (a) Pot. trioxalatoferrate (III)
  - (b) Pot. trioxalatochromate (III)
  - (c) Diaquodioxalatochromate (III)
  - (d) Hexaminenickel (II) chloride

50 Marks

4. Viva-Voce 10 Marks

5. Record of Practical Note Book

10 Marks

# SUGGESTED BOOKS:

 Vogel's Text book of Qualitative Chemical Analysis by J. Bassett, G. H. Jeffery and J. Mendham, ELBS.

2. Vogel's Text Book of Quantitative Chemical Analysis. 5<sup>th</sup> Editionby J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical.

3. Inorganic Semimicro Qualitative Analysis by V. V. Ramanujam. The National Pub. Co.

4. Practical Inorganic Chemistry by G. Marr and B. W. Rockett, Von Nostrand Reinhold

Co., London.

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# M.Sc. (Chemistry) Semester-III M-Chem-301 Chemical Spectroscopy

Time - 3 Hours			Full Marks: 70
	Part-A		
Ten Multiple Choice Questions (Compu	ilsory)		10 x 2=20 Marks
(Two Questions from each unit)			
	Part-B		
Five Short Answer Question (Four to be	Answered)		4 x 5=20 Marks
(One Question from each unit)			
	Part-C	~	
Three Long Answer Question (Three to	be Answered)		10 x 3=30 Marks
(One Question from each unit)			

### Unit I: Rotational and Vibrational spectroscopy

**Molecular spectroscopy:** Born-Oppenheimer approximation, Regions of electromagnetic spectrum and associated spectroscopic techniques, Heinsenberg's Uncertainty principle, Basic elements of spectroscopy, natural line width and natural line broadening, transition probability, Time-dependent perturbation, transition moment, selection rules, Lambert-Beer's law.

Rotational Spectra: Rigid rotor model, non-rigid rotators, quantization of rotational energy level, fine structure of rotational spectra, isotope effect, first order Stark effect, nuclear and electron spin interaction, bond length calculation. Classification of polyatomic molecules, Energy level and spectra of symmetric top molecules and asymmetric top molecules, criterion for absorption of radiation-selection rule.

Vibrational Spectra: Schrodinger equation for harmonic oscillator, quantization of vibrational energy levels, vibrational energies of diatomic molecule, zero point energy, force constant and bond strength, Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation, anharmonic oscillator, overtones and combination bands, Dissociation energies from vibrational data, Morse potential energy diagram, vibrational-rotational spectroscopy, P,Q,R branches, Breakdown of Born-Oppenheimer approximation, Vibrations of polyatomic molecules, selection rules, normal modes of vibrations, group frequencies, hot bands, factors affecting band positions and intensities, normal co-ordinate analysis, symmetry for normal co-ordinates (use of group theory).

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Raman spectroscopy: Concept of polarizability, Pure rotational, vibrational and rotational-vibrational spectra, Stokes and anti-Stoke's lines- Selection rules. Advantages of Raman spectroscopy over IR spectroscopy, Selection rules for IR spectra and Raman spectra, group frequencies, overtones, polyatomic molecules, normal modes of vibration, finger print region, mutual exclusion principle and coherent anti-stokes Raman spectroscopy (CARS). Symmetry, shapes and molecular vibrations of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub>.

### Unit II: Electronic Spectroscopy

Energy of atomic orbitals, vector representation of momentum and vector coupling spectra of H- atom, Energy levels, Molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon Principle,, Breakdown of selection rules, electronic spectra of polyatomic molecules, Dissociation energies, photoelectron spectroscopy of diatomic molecules and simple polyatomic molecules, Phosphorescence and florescence Adiabatic and vertical ionization energies,

Polyatomic molecules, oscillator strengths, use of free electron model, HMO theory and group theory for polyenes and carbonyl compounds, qualitative ideas of solvent effects-viscosity, polarity and hydrogen bonding. Excited states, Jablonskii diagram, Florescence and phosphorescence, Quenching, Stern-Volmer equation.

#### Unit III: NMR Spectroscopy

Nuclear spin, nuclear resonance, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical de-shielding, spin-spin interactions, factors influencing coupling constant, NMR studies of nuclei other than proton(<sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P).

Larmor precession, Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation, quantum mechanical treatment of AB system, Selection rules and relative intensities of lines, Nuclear Quardrupole Reasonance (NQR) spectra and its application.

- (a) Application of NMR Spectroscopy: Shielding mechanism, chemical shift values and correlation for protons bonded to carbon and other nuclei, chemical exchange, spin-spin interaction. Interpretation of PMR spectra of organic compounds.
- (b) Carbon-13 NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, acetylenic, aromatic, heteroaromatic and carbonyl carbons), Coupling constant.

# Unit IV: Application of Spectroscopy:

(a) UV and Visible Spectroscopy- Various electronic transitions, Beer- Lambert law, effect of solvent on electronic transitions, Fischer-Woodward rules for conjugated dienes and carbonyl compounds, UV spectra of aromatic and heterocyclic compounds, steric effects in histographs.

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(b) IR Spectroscopy: Characteristic vibrational frequencies of organic functional groups, detailed study of vibrational frequencies of carbonyl compounds, effect of H-bonding and solvent effect on vibrational frequencies.

Unit V: Mass Spectrometry: Ion production, factors affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, Example of mass spectral fragmentation of organic compounds with respect to their structure determination.

# SUGGESTED BOOKS:

- 1. Modern Spectroscopy: 4<sup>th</sup> Ed. by Hollas, J.M., John Wiley & Sons.
- 2. Introduction to Molecular Spectroscopy by Barrow, G.M. McGraw-Hill, N.Y.
- 3. Basic Principles of Spectroscopy by Chang, R. McGraw-Hill, N.Y.
- 4. Physical Methods in Chemistry by Drago, R.S.
- 5. Introduction to Molecular Spectroscopy by Banwell, C.N.
- 6. Introduction to NMR Spectroscopy by Abraham, R.J., Fisher, J. and Coftus, P. Wiley.
- Application of Spectroscopy to Organic compounds by Dyer, J.R.Prentic Hall.
- 8. Organic Spectroscopy by Kemp, W. John Wiley.
- 9. Introduction to Spectroscopy by Pavia, Donald L.
- 10. Modern NMR, techniques for Chemistry Research by Derome, A.E. Pergamon.
- 11. Spectroscopic Methods in Organic Chemistry by Williams, D.H. and Flaming, I: Tata McGraw Hill.
- 12. Chemical Application of Group Theory by Cotton, F.A. Wiley.

13. Organic Spectroscopy by V.R. Dani, Tata McGraw Hill.

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# M.Sc. (Chemistry) Semester-III M-Chem - 302

### Environmental, Analytical and Bio - inorganic chemistry

11me - 3 Hours			Full Marks: 70
	Part-A		
Ten Multiple Choice Questions (Con	npulsory)		10 x 2=20 Marks
(Two Questions from each unit)			
	Part-B		
Five Short Answer Question (Four to	be Answered)		4 x 5=20 Marks
(One Question from each unit)			
	Part-C	~	
Three Long Answer Question (Three	to be Answered)		10 x 3=30 Marks
(One Question from each unit)			

#### Unit I: Environmental Chemistry

- a) Introduction to Environmental Chemistry: Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments. The natural cycles of environment (Hydrological, Oxygen, Nitrogen, Phosphorous and Sulphur cycles).
- b) Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in the atmosphere, stratospheric chemistry: The chemistry of ozone layer, The role of chemicals in ozone destruction, The green-house effect and Global warming, El-Nino phenomenon.
- c) Hydrosphere: Complexation in natural water and waste-water, Micro-organism in aquatic chemical reactions, Eutrophication, Re-cycle of waste-water in process industry, Treatment of sewage and reuse of water in industry and agriculture, Microbiologically mediated redox reactions and Nitrogen transformation by bacteria.
- d) Lithosphere: The terrestrial environment, Soil formations, Soil properties (physical/chemical), inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil, waste and pollutants in soil, waste classification and disposal.
- e) Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide,

nitrogen oxides, sulphur oxides, ozone, PAN, cyanide, pesticides, insecticides and carcinogens.

#### Unit II: Pollution

- a) Air Pollution: Air pollutants (sources, classification, sampling and monitoring): Particulates, Aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon emission, Photochemical reaction, smog, Auto-exhausts, Acid-rains, Air-quality standards.
- b) Water Pollution: Water pollutants (sources, sampling and monitoring), Water-quality parameters and standards: physical and chemical parameters (colour, odour, taste and turbidity), Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation.
- c) Industrial Pollution: Cements, Sugar, distillery, drug, paper and pulp, thermal power plants, metallurgy, polymers, disposal of industrial waste and their management.
- d) Environmental Management: Methods of environmental management, Radioactive waste management, Environmental impact assessment, Natural resources of energy-consumptions and conservation.

#### Unit III: Analytical Chemistry

- a) Separation Methods: Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography (HPLC).
- b) Thermal Analysis: Theory, methodology and applications of thermo gravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.
- c) Colorimetry: Basic principles, Beer-Lambert law, photoelectric colorimeter and its application for the estimation of carbohydrates, ascorbic acid and proteins.

#### Unit IV: Chromatography

Basic principles, classification, chromatography terminology ( $R_f$  value), Liquid – Gas chromatography, ion–exchange chromatography, stationary and mobile phase chromatography.

#### Unit V: Bio-Inorganic Chemistry

Fundamental of inorganic biochemistry, essential and non – essential element in bio – systems, role of alkali/alkaline earth metals in bio – systems. Role of metal ions in oxygen

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carriers and synthetic oxygen carriers. Fixation of dinitrogen biologically and abiologically. Metal ions as probes for locating actives sites, antioxidants, metal ions as antioxidants, metal ion enhancing catalytic activity of enzyme (Biocatalyst), metalloproteins. Metal complexes of polynucleotides, nucleic acids (DNA & RNA). Role of metal ions in replication and transcription process of nucleic acids. Bioinorganic chips and biosensors.

## SUGGESTED BOOKS:

- 1. Environmental Chemistry: A Global Perspective by G.W. Vanloon, S.J. Duffer,Oxford University Press.
- 2. Environmental Analytical Chemistry by F.W. Fifield and W.P.J. Hairens, Black Well Science.
- 3. Environmental Chemistry by Colin Baird, W.H. Freeman and Company, New York.
- 4. Environmental Chemistry by A.K. De, New Age International Private Ltd., New Delhi.
- 5. Principles & Techniques by L.G. Hargis, Prentice Hall.
- 6. Principles of Instrumental analysis by D.A. Skoog and J.L. Loary.
- 7. Analysis of Air Pollutants by Peter O. Warner, John Wiley, New York.
- 8. Environmental Pollution Analysis by S.M. Khopkar, Wiley Estern Ltd., New Delhi.
- 9. Environmental Chemistry by S.K. Banerji, Prentice-Hall of India, New Delhi.
- 10. Principles of Instrumental Analysis by D.A. Skoog, Saunders College Publishing, Philadelphia, London.
- 11. Modern Methods of Chemical Analysis by R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William. John Wiley, New York.
- 12. Principles of Analytical Chemistry by J.H. Kennedy, Saunders Holt, London.

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Time - 3 Hours Full Marks: 70

Part-A

Ten Multiple Choice Questions (Compulsory) 10 x 2=20 Marks

(Two Questions from each unit)

Part-B

Five Short Answer Question (Four to be Answered) 4 x 5=20 Marks

(One Question from each unit)

Part-C

Three Long Answer Question (Three to be Answered) 10 x 3=30 Marks

(One Question from each unit)

Unit I: Metal ions in Biological system- Essential and trace metals, Role of metal ions (Ca,Mg,Fe,Na,K) in biological process, metal complexes in transmission of energy-Chlorophyll, Photosystem I and photosystem II in cleavage of water system.

Natural Oxygen carrier - Haemoglobin, Myoglobin, Hemicyanin and Hemierythritin. Synthetic oxygen carrier- complex of Cobalt and Iron, Cytochrome P<sub>450</sub>, cytochrome-C, Rubredoxins and ferrodoxins, Copper blue proteins, Non haeme proteins-ferritin and transferrin, metalozyms, fixation of nitrogen. Haeme proteins and oxygen uptake, structure and functions of Haemoglobin, Myoglobin and Hernicyanin.

Unit II: Enzymes' Properties—Specificity, enzyme kinetics, Michaelis-Menton equation, steady state kinetics, inhibition, Transition state theory, orientation and steric effect. Coenzymes- cofactors as derived from Vitamins, prosthetic groups, thiamine pyrophosphate, pyridoxal phosphate, NAD, NADP, FMN, FAD, lipoic acid and Vit. B12.

**Unit III:** Bioenergetics - Standard Free energy change in biochemical reactions, hydrolysis of ATP, synthesis of ATP, entropy change in biological process. Structure and functions of cell membrane, Ion transport through cell membrane.

Unit IV: Carbohydrade metabolism- Calvin cycle, Krebs cycle, Glycolysis, glucogenesis, glycogenolysis, biosynthesis of disaccharides and polysaccharides. Pentose phosphate

pathway (PPP).

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# Unit V: Protein Synthesis and Nucleic Acid

- (a) Protein: Strategy of peptide bond synthesis. Protection of -NH<sub>2</sub> and activation of -COOH groups of amino acids. Amine protecting groups: tert-Butoxycarbonyl (t-BOC), benzyloxycarbonyl (Carbobenzoxy, Cbz), (9-Fluoronyl)-methoxycarbonyl (Fmoc). Deprotection of blocking groups. Condensing agent DCC (Dicyclohexylcarbodiimide). Illustartion of peptide synthesis. Solid-phase peptide synthesis.
- (b) Nucleic Acids: Methods of determining base sequence of DNA: Sanger's dideoxy method, autoradiography. Concept of restriction enzyme, recombinant DNA technology. Synthesis of mono and oligo nucleotides. Laboratory synthesis of DNA strand. Basic idea of DNA fingerprinting and its applications.

# SUGGESTED BOOKS:

- 1. Concise Text Book of Biochemistry by T. N. Pattabhiraman, All India Publishers.
- 2. Biochemistry by A. L. Lehninger. al., CBS.
- 3. A Text Book of Biochemistry by A. V. S. S. Rama Rao, UBSPD.
- 4. Biochemistry by P. C. Champe and R. A. Harvey, J. B. Lipincott & Co.
- 5. Fundamentals of Biochemistry by J. L. Jain, S. Chand & Co.
- 6. Biochemistry by COSIP-ULP, Bangalore University.
- 7. Outlines of Biochemistry by Conn E. E and Stumpf P. K., John Wiley & Sons.
- 8. General Biochemistry by Weil J. H., Wiley Eastern
- 9. Biochemistry by Campbell M. K., Harcourt Brace & Co.
- 10. Principles of Biochemistry by Voet & Pratt.
- 11. Illustrated Reviews of Biochemistry by Harper.
- 12. Biochemistry by Stryer.

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# M.Sc. (Chemistry) Semester-III M-Chem-304 Organic Lab course

Time – 6 Hours

Full Marks: 70

- 1. Systematic analysis and identification of organic compounds.
- 2. 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
- 3. Anthranilic acid from phthalic acid.
- 4. Benzanilide from benzophenone.
- 5. Benzilic acid from benzoin.
- 6. Synthesis of Acridone.
- 7. Synthesis of Hydantoin.
- 8. Titrimetric estimation of amino acids.
- 9. Saponification value of oil.
- 10. Estimation of glucose by Feighling's method.
- 11. Estimation of Keto group.
- 12. Estimation of phenols.
- 13. Iodine value of oil (chloramine-T method).

50 Marks

14. Viva-Voce

10 Marks

15. Record of Practical Note Book

10 Marks

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#### SUGGESTED BOOKS:

- 1. Laboratory manual of Organic Chemistry by B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi.
- 2. Practical Organic Chemistry by Mann and Saunders.
- 3. Text Book of Practical Organic Chemistry by A. I. Vogel.
- 4. Test Book of Quantitative Organic Analysis by A. I. Vogel.
- 5. A Handbook of Organic Analysis by Clarke and Hayes.
- 6. Comprehensive Practical Organic Chemistry: Preparation and quantitative Analysis by V. K. Ahluwalia, R. Agarwal, Universities Press (India).
- Comprehensive Practical Organic Chemistry: Qualitative analysis by V. K. Ahluwalia, S. Dhingra, Universities Press (India).
- 8. An advanced course in Practical chemistry by A. Ghoshal, and B. Mahapatra New Central Book Agency, Calcutta.
- Advanced Practical Organic Chemistry (Vol I and II) by J. Mohan, Himalaya Publishing House.
- Practical Organic Chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi.

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# M.Sc. (Chemistry) SEMESTER- IV

# M-Chem 401(A) - Elective Physical Advanced Statistical Thermodynamics

Time – 3 Hours	Full Marks: 70
Part-A	
Ten Multiple Choice Questions (Compulsory)	10 x 2=20 Marks
(Two Questions from each unit)	
Part-B	
Five Short Answer Question (Four to be Answered)	4 x 5=20 Marks
(One Question from each unit)	
Part-C	
Three Long Answer Question (Three to be Answered)	10 x 3=30 Marks
(One Ouestion from each unit)	

#### Unit I: Advanced Statistical Mechanics

Statistical Thermodynamics: Foundation of Molecular thermodynamics ensemble, ensemble average, micro-canonical ensemble, canonical and grand canonical ensemble, ideal gas in canonical ensemble, comparison of various ensembles.

**Types of Statistics:** Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Derivation of the equations for above three distribution Laws. Comparison of Bose-Einstein and Fermi-Dirac statistics with Maxwell-Boltzmann statistics.

Applications to Ideal Gases: Thermodynamic probability; Most probable distribution Law, Partition Function (Definition and significance), Partition functions: translational, rotational, vibrational partition function for monoatomic, diatomic and polyatomic gases, Molecular partition function; electronic and nuclear partition functions. Statistical definition of entropy. Ortho and para hydrogen and their Statistical ratio. Theories of heat capacity of solids: Specific heat of solids, Einstein's theory and Debye Theory of heat capacity of Solids.

# Unit II: Theory of imperfect gases and condensation

Partition functions and cluster integrals; pressure of gas expressed as power series in activity; irreducible cluster integrals; Virial expansion for a gas; theory of condensation.

# Unit III: Theory of liquids

Canonical Ensemble: Definition of distribution and correlation functions; Thermodynamic Function of Fluids and radial distribution functions; Fluid with modified Lennard Jones Molecular Interaction potential according to the superposition approximations.

Grand Canonical Ensemble: Distribution functions in monoatomic, one component systems;

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Kirkwook-Salsburg integral equation.

## Unit IV: Lattice statistics

Nearest neighbor lattice statistics-thermodynamics and interconnections; Exact and formal methods.

# Unit V: Irreversible Thermodynamics/ Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states-Phenomenological Laws and Onsager's reciprocity relations, entropy production, Excess entropy production, local entropy and entropy flow. Rate of entropy production; entropy balance equations for different irreversible processes; Transformations of the generalized fluxes and forces. Phenomenological relations theorem of minimum entropy production; electro kinetic phenomena; diffusion; electric conduction; irreversible thermodynamics of biological systems; coupled reactions.

#### SUGGESTED BOOKS:

- 1. Physical Chemistry by P. Atkins and J. D. Paula, 9th Ed., Oxford University Press.
- 2. Quantum Chemistry by D.A. McQuarrie Viva, New Delhi.
- 3. Quantum Chemistry by J.P. Lowe & K. Peterson, Academic Press.
- 4. Elementary Quantum Chemistry by F.L., Pilar, Dover Publication, N.Y.
- Principles of Quantum Chemistry by Ram Yatan Prasad, Foundation Books, New Delhi 2015.
- 6. Introduction to Quantum Chemistry by A. K. Chandra, Tata McGraw Hill.
- 7. Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey.
- 8. Quantum Chemistry by R. K. Prasad, New Age International.
- 9. Quantum Chemistry through problems and solutions by R. K. Prasad, New Age International.

 Introduction to Thermodynamics of Irreversible Processes by Prigogine Ilya, New York: Interscience Publishers.

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# M.Sc. (Chemistry) Semester - IV

# M-Chem 402 (A) - Elective Physical Advanced Chemical Reaction Dynamics

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	~	10 x 3=30 Marks

# Unit I: Introduction to Advanced Chemical Dynamics:

(One Question from each unit)

Dynamics of reaction, mechanism of activation, concept of shape of energy surfaces, rate of reaction on theoretical potential energy surfaces, determination of position and properties of the transition state on surfaces.

# Unit II: Kinetics of condensed phase reaction and statistical theory of kinetics:

Transition State Theory: Application of statistical mechanics to transition state theory, Comparison of transition state theory with experimental results. Thermodynamic treatment of TST. Theories of unimolecular reactions--treatments of Lindmann, Hinshelwood, Rice-Ramsperger-Kassel (RRK), and Rice-Ramsperger-Kassel-Marcus (RRKM).

# Unit III: Catalysis and Oscillatory Behaviors:

Mechanism and kinetics of catalytic reaction. Arrhenius intermediate, Van't Hoff intermediate. Theory of acid and base catalyst and effect of salt on acid base catalysis. Bronsted catalysis law, linear free energy relationship. Hammet equation, oscillatory reaction, Lotka-Volta model, B-Z reactions and its mechanism.

#### Unit IV: Study of Fast Reactions and Enzyme Kinetics:

Flow techniques, relaxation methods, flash photolysis, NMR method, Molecular beam and Shock tube kinetics, stop flow method, Photo dissociation and recombination reactions. Kinetics of enzyme action - Michaelis-Menton equation. Different plots for determination of

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 $K_m$  and  $V_{max}$  and their physiological significance. Two substrate reactions; Enzyme inhibition-reversibility and product inhibition.

# Unit V: Corrosion and Advanced Electrochemistry

Corrosion: Scope and economics of corrosion, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), units of corrosion rate, passivity and its breakdown, Corrosion prevention (electrochemical, inhibitor, and coating methods).

Cyclic Voltammetry: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry, interpretation of voltammograms. Kinetics of electrode reactions, faradaic and non-faradaic current, rate law in faradaic process, current density, factors affecting electrode reaction rate, Nernst diffusion layer, exchange current density, effect of double layer structure on electrode reaction-rate.

#### SUGGESTED BOOKS:

- Reaction Kinetics by M. J. Pilling and A.P.W, Seakins, Oxford Science Publication, New York.
- 2. Chemical Kinetics by K.J. Laidler, Harper & Row Publishers, New York.
- Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, MacMillan India Ltd., New Delhi.
- 4. Modern Liquid Phase Kinetics by B. G. Cox, Oxford University Press, Oxford.

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## M.Sc. (Chemistry) Semester- IV M-Chem 403 (A) - Elective Physical Advance Quantum Chemistry

Time – 3 Hours

Part-A

Ten Multiple Choice Questions (Compulsory)

(Two Questions from each unit)

Part-B

Five Short Answer Question (Four to be Answered)

(One Question from each unit)

Part-C

Full Marks: 70

10 x 2=20 Marks

4 x 5=20 Marks

Three Long Answer Question (Three to be Answered)

10 x 3=30 Marks

(One Question from each unit)

## Unit I: Elementary Matrix Theory and Matrix Operator:

Review of matrix algebra and angular momentum, projection operator, matrix representation of Schrödinger wave equation.

Similarity transformation and block diagonalization of matrices. Matrix transformation of linear equation.

## Unit II: Perturbation Theory and Approximation method:

Perturbation theory for degenerate states. Double pertubation theory. Many electron systems. Concept of spin and determinantal wave function, qualitative treatment of Hartree-Fock theory, SCF procedure, SALC, orbital and spin angular momentum operators. Pauli Matrices. Term symbols and term energies.

## Unit III: Semi-Empirical Theories:

Treatment of HMO, EHT and PPP method. ZDO approximation, CNDO, INDO and other semi-empirical theories. Roothan equation, Koopman and Brillouin theorem.

## Unit IV: Density Function Theory:

Hohenberg-Kohn theorem. Kohn-Shan energy. The Kohn-Shan equation, Local Density Approximation (LDA). Evaluation of group electronegativity and hardness & Softness of group 14 elements in periodic table (C, Si, Gi, Sn, Pb).

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## Unit V: Basis Sets:

Slater, Gaussian and Integral transformation, Basis set Superposition Error (BSSE). Electron Correlation (EC) and Confugration Intraction (CI) theories.

## SUGGESTED BOOKS:

- 1. Physical Chemistry by P. Atkins and J. D. Paula, 9th Ed., Oxford University Press
- 2. Quantum Chemistry by D.A. McQuarrie Viva, New Delhi.
- 3. Quantum Chemistry by J.P. Lowe & K. Peterson, Academic Press.
- 4. Elementary Quantum Chemistry by F.L., Pilar, Dover Publication, N.Y.
- 5. Principles of Quantum Chemistry by Ram Yatan Prasad, Foundation Books, New Delhi
- 6. Introduction to Quantum Chemistry by A. K. Chandra, Tata McGraw Hill.
- 7. Quantum Chemistry by Ira N. Levine, Prentice Hall, New-Jersey.
- 8. Quantum Chemistry by R. K. Prasad, New Age International.

9. Quantum Chemistry through problems and solutions by R. K. Prasad, New Age International.

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## M. Sc. (Chemistry) Semester- IV M-Chem-404 (A) Elective Physical Lab course

### Time - 6 Hours

#### Full Marks: 70

#### **Chemical Kinetics**

- 1. Determination of Temperature Coefficient and Energy of Activation of the hydrolysis of ethyl acetate.
- 2. Determination of order of reaction of Persulphate Iodide Reaction.
- 3. Effect of ionic strength on the rate of Persulphate- Iodide Reaction.
- 4. Kinetics of oxidation of Alcohol by Potassium Dichromate using Spectrophotometer.
- 5. Determination of rate constant of inversion of Sucrose (Cane sugar) by acid using Polarimeter.
- 6. Analysis of a mixture of Sucrose. Dextrose and Fructose using Polarimeter.

### Conductometry

- 7. Verification of Onsager Equation and Determination of Equivalent Conductance of strong electrolyte at infinite dilution.
- 8. Determination of Critical Micelles Concentration (CMC).
- 9. Thermodynamic Parameters of a cell reaction by EMF measurement.
- 10. Determination of Solubility Product (KSP) of AgCl.
- 11. Determination of Hydrolysis Constant and Degree of Hydrolysis by
  - (a) titration of strong / weak acid with strong base,
  - (b) titration of a mixture of strong acid and weak acid with strong base.

## Photometry, Adsorption, Refractometry and Molar Volume

- 12. Verification of Beer and Lambert Law.
- 13. Simultaneous estimation of Manganese and Chromium in a mixture of Potassium Dichromate and Potassium Permanganate solution.
- 14. To determine the composition of a complex using Spectrophotometer. (Job Continuous Variation Method).
- 13. Determination of Adsorption Isotherm for the Adsorption of acetic acid and oxalic acid on active charcoal by Graphical Method.
- 14. Determination of very low Concentration of Metals in solution by Flame Photometer.
- 15. Determination of Specific and Molar Refraction of a liquid by using Refractometer.
- 16. Determination of Partial Molar Volume of Ethanol Water Mixture.

### **Distribution Law**

17. Calculation of Degree of Association of Benzoic Acid.

18. Calculation of Molecular Formula of Copper - ammonia complex by using the Partition Coefficient Method.

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19. To study of Distribution Coefficient of iodine between Water and carbon tetrachloride and then determine the equilibrium constant for the reaction KI + I<sub>2</sub>= KI<sub>3</sub> by Partition Method.

## Potentiometetry, Thermochemistry and Colloids

- 20. Determination of Dissociation constant of weak acid by Potentiometric Titration.
- 21. Redox Titration of Potassium Dichromate versus Ferrous Sulphate.
- Precipitation Titration of a Mixture of Chloride, Bromide and Iodide with Silver Nitrate solution.
- 23. Determination of Precipitation Values of NaCl, BaCl<sub>2</sub>, AlCl<sub>3</sub> and As<sub>2</sub>S<sub>3</sub>Sol.
- 24. Determination of Isoelectric Point of Lyophilic Sol
- 25. Determination of water Equivalent of a calorimeter and heat of Displacement for the reaction:  $Cu^{2+} + (aq) + Zn(s) = Zn^2 + (aq) + Cu(s)$ .

  50 Marks

26. Note-Book

10 Marks

27. Viva-voce

10 Marks

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#### SUGGESTED BOOKS:

- 1. Findlays Practical Physical Chemistry (rev.) by P. B. Levitt, Longman's London.
- Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Ed.
- 3. Practical Physical Chemistry by B. Viswanathan & P.S. Raghwan: Viva Books Pvt. Ltd., New Delhi.
- 4. Experiments in Physical Chemistry by J.C. Ghosh, Bharti Bhawan, Patna.
- 5. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut
- 6. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi.
- 7. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York.
- 8. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd.
- 9. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York.
- 10. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi.
- 11. Experimental Physical Chemistry by V. D. Atavale and ParulMathur, New Age International, New York.
- 12. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co .new York.

13. Practical's in Physical Chemistry: A Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi.

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## M.Sc.(Chemistry) Semester- IV M-Chem 401(B) - Elective Inorganic Ligand Field Theory

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	~	10 x 3=30 Marks
(One Ouestion from each unit)		

## Unit I: Multiple and fine structure in Atomic spectra

Free ion terms, Hunds rule, L-S and J-J coupling schemes, Condon and Shortly parameters, Racah parameters, Lande internal rules, Multiplet separation, spin orbit coupling constant. Van-Vleck susceptibility equation and its application, TIP effect on spin orbit coupling, electron delocalization on magnetic properties, anti-ferromagnetic exchange interaction.

#### Unit II Metal ions in Chemical Environment:

Splitting of terms in  $O_h$ ,  $T_d$  and  $D_{4h}$  symmetry, Transformation properties of s,p,d orbitals in chemical environment by the use of character table , Sine formula and its derivations; strong field configuration, strong field components, Non crossing rules, Correlation diagram for  $d^2$ ,  $d^3$  and  $d^8$  system in cubic symmetry, cross over points, T-S diagram.

## Unit III M.O. Description for bonding in Co-ordination Compounds:

Classification of ligand as sigma and pi donor ligands, pi acceptor ligands, symmetry consideration of metal orbitals and ligand group orbitals in O<sub>h</sub> point group for sigma and pi bond formation, use of character table for formation of M.Os in O<sub>h</sub> and T<sub>d</sub> point group with and without pi bonding, MO energy level diagram.

## Unit IV: Absorption Spectra and other spectroscopic evidences for ligand field effect

Band assignment, determination of ligand field splitting parameters, Nephalauxetic ratio, Jahn Teller distortion, Vibronic coupling, spin-orbit coupling, C T Bands and their assignment.

Application of IR in metal carbonyls, nitrosyls, linkage isomerism, mode of metal ligand bonding.

## Unit V: Modern Spectroscopy

- (a) NMR spectra of paramagnetic transition metal complexes, contact shift and pseudo contact shift.
- **(b)** ESR Principle of ESR spectroscopy, presentation of spectrum, theory of hyperfine interaction, isotopic g and A values, anisotropy, zero field splitting, application to transition metal complexes.
- (c) Mossbauer spectra: Mossbauer effect, recoil energy and X-ray emission, isomer effect, magnetic hyperfine interaction, application of spectra to Fe (57) and I (129) compounds.

### SUGGESTED BOOKS:

- 1. Physical Methods in Chemistry by Drago, R.S. W.B. Saunders co. U.K.
- 2. Infrared and Raman Spectra Inorganic and co-ordination Compounds by Nakamoto Kazuo, John Wiley & Sons.
- 3. Inorganic Chemistry, Principles and Structures and Reactivity by James E. Hubeey.
- 4. Co-ordination Compounds by S.F.A Kettle, ELBS.
- 5. Electronic Spectra of Transition Metal Complexes by D. Sutton; Mc Graw-Hill, New York.
- Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson, John Wiley & Sons, New York.

7. Introduction to Ligand Field Theory by C.J. Ballhausen; McGraw Hill Books Co., N.Y.

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## M.Sc. (Chemistry)

### Semester- IV

## M-Chem 402(B) - Elective Inorganic Reaction Mechanism & Supramolecular Chemistry

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	~	10 x 3=30 Marks
(One Question from each unit)		

**Unit I: Electron-transfer reaction:** Outer sphere and inner sphere mechanism, Marcus-Hush theory, complementary and non-complementary reactions, mixed valence complexes and their electron transfer model.

**Unit II: Molecular rearrangements:** D and A process, reactions of geometrical and optical isomers, optical inversion, isomerism and racemerisation of octahedral complexes, intramolecular rearrangement.

**Unit III: Photochemistry of metal complexes:** Basis of photochemistry, properties of excited states, excited states of metal complexes and their comparison with organic compounds; photo substitution, photo oxidation and photo reduction and excited electron transfer. Reactions of 2, 2- bipuridines and 1, 10- phenanthroline complexes, metal complex sensitisers, photochemistry of Co (III) and Cr (III) complexes. Applications of photochemical reactions of coordination compounds.

Unit IV: Supramolecular Chemistry: Introduction, some examples of self-assembly in supramolecular chemistry, reactivity and catalysis design and synthesis.

Unit V: Metal Alkoxides: Synthesis, structure, bonding and application of metal alkoxides, metal acetylacetonates Schiff base metal complexes.

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## SUGGESTED BOOKS:

- 1. Chemistry of Metal Chelate Compound by A.E. Martell & M Calvin, Prentice-Hall.
- 2. Advance Inorganic Chemistry by F.A. Cotton & G. Wilkinson
- 3. Aspects of Organic Photochemistry by W.M. Horspool, Academic Press, New York.
- 4. Photochemistry of Coordination Compounds by V. Balzani and V. Carassiti, Academic Press, London.
- 5. Supramolecular Chemistry: Concepts and Perspectives by J.M. Lehn, Wiley-VCH.
- 6. Perspective in supramolecular Chemistry: Vol. 2- Crystal Engineering and Molecular Recognition by G.R. Desiraju, Wiley: Chichester.
- 7. Supramolecular Chemistry: A Concise Introduction by J.L. Atwood & J.W. Steed, John Wiley& Sons.

8. Concepts of Inorganic Photochemistry by A.W. Adamson & P.D. Fleiscauer (Eds), N.Y.

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## M.Sc.(Chemistry) Semester- IV M-Chem 403 (B) - Elective Inorganic Organometallics and Metal Clusters

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	~	10 x 3=30 Marks

## Unit I: Transition Metal-Carbon σ-bonded compounds:

Introduction to organometallics,  $\sigma$ -alkyl and aryl compounds with transition metals and their synthesis, structure and reactivity, organocopper in organic synthesis.

## Unit II: Transition Metal-π complexes:

(One Question from each unit)

Alkyne, allyl, Alkene, Diene, Dienyl, arene and trienyl complexes of transition metals and their preparation, properties, nature of bonding and structural features, Important reactions related to nuclephilic and elecrophilic attack

## Unit III: Catalysis of Organometallic Compounds:

Oxidative addition and reductive elimination processes, catalytic reactions of olefin-hydrogenation using Wilkinson catalyst, isomerization, hydroformylation (Oxo-processes and Repe reaction) by cobalt and rhodium catalyst, Wacker process, polymerization (Using Zeigler-Natta process), Oligomerisation, Fischer- Tropsch reaction and water gas reaction, activation of C-H bond.

## Unit IV: Metal-Metal Bond and Metal Clusters:

Metal-Metal multiple bonds, major structural type, relation with clusters, one dimensional solids, classification, structures and electron count in  $M_3$ ,  $M_4$  and  $M_5$  clusters, LNCC and HNCC structures, Isolobal and Isoelctronic relationship.

## Unit V: Metal - Hydrogen Complexes:

Hydrogen bonded transition metals complexes, Fluxional organometallic compounds.

## SUGGESTED BOOKS:

- Principles of Organometallic Chemistry by M.L.H Green, G.E. Coates & P.Powell: Chapman & Hall, U.K.
- Organometallic Reagents in Synthesis by P. R. Jenkins, Oxford Science Publication, Oxford.
- Principles and Applications of Organotransition Metal Chemistry by J. P. Collman, L. S. Hegedus, J. R. Norton and Richard G. Finke, University Science Books, Mill Valley, California.
- 4. The Organometallic Chemistry of the Transition Metals by R.H. Crabtree, John-Wiley & Sons, New York.
- 5. Organometallic Chemistry by R. C. Mehrotra and A. Singh; New age international.
- 6. The Organometallic Chemistry of transition metals by R. H. Crabtee; John Wiley.
- 7. Organometallic Chemistry by ch. Elschewbroich and Slazer, VCH.
- 8. Organometallics (Vol. 1 & 2) by M. Bochmann, Oxford Chemistry Primers, Oxford University.
- 9. Catalytic Chemistry by B. C. Gates; John Wiley and sons.
- Applied Organometallic Chemistry and Catalysis by Robin Whyman, Oxford University Press.
- 11. Basic Organometallic Chemistry by B. D. Gupta and A. J. Elias, University Press,
- 12. Heterogeneous Catalysis by D. K. Chakraborty and B. Viswanathan, New Age International.
- 13. Organometallics (Vol. 1 & 2) by M. Bochmann, Oxford Chemistry primers, Oxford University Press.
- 14. Organotransition Metal Chemistry by Y S. G. Davies, Pergamon Press, Oxford.

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# M.Sc. (Chemistry) Semester- IV M-Chem 404 (B) Elective Inorganic Lab course

Time - 6 Hours

Full Marks: 70

- 1. Systematic qualitative analysis of inorganic mixture containing at least six radicals including Cr, Mo, W, Mn, Ce.
- 2. a) Use of EDTA in volumetric analysis
  - b) Analysis of at least two metal ion in alloys and minerals (Bauxite, dolomite, hematite, steel, brass and common solder)
- 3. Preparation of complex compounds of Iron, Chromium and Copper.

50 Marks

4. Note-Book

10 Marks

5. Viva-voce

10 Marks

## SUGGESTED BOOKS:

- 1. Vogel's Text book of Qualitative Chemical Analysis by J. Bassett, G. H. Jeffery and J. Mendham, ELBS.
- 2. Vogel's Text Book of Quantitative Chemical Analysis by J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical.
- 3. Inorganic Semi micro Qualitative Analysis by V. V. Ramanujam; The National Pub. Co.

4. Practical Inorganic Chemistry by G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London.

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10 x 3=30 Marks

## M.Sc.(Chemistry) Semester- IV M-Chem-401 (C) Elective Organic Organic synthesis

Time - 3 riours	Full Marks: 70
Part-A	
Ten Multiple Choice Questions (Compulsory)	10 x 2=20 Marks
(Two Questions from each unit)	
Part-B	
Five Short Answer Question (Four to be Answered)	4 x 5=20 Marks
(One Question from each unit)	

Unit I:

(One Question from each unit)

(a) Organometallic Reagents: Principles, preparation, properties and application of the following (with mechanistic details) - Li, Mg, Cd, Zn, Cu, Sn, Si and B organometallics.

Part-C

Three Long Answer Question (Three to be Answered)

**(b) Organopalladium Chemistry:** Basic knowledge of the following coupling reactions: Stille reaction, Suzuki reaction, Sonogashira reaction and Heck reaction.

### Unit II:

- (a) Oxidation: Different oxidative processes: Oxidation of alkenes, aromatic hydrocarbons, allylic alcohols, diols and ketones, with emphasis on oxidation by per acids, peroxides,HIO<sub>4</sub>, Pb(OAc)<sub>4</sub> and SeO<sub>2</sub>. Protection and deprotection of the following functional groups: hydroxy (alcohols and diols), amino, carbonyl & carboxyl groups (with mechanism, regioselectivity, chemoselectivity and sterioselectivity).
- (b) Reduction: Different reductive processes: Reduction of alkenes, alkadienes, alkynes, aromatic rings, different carbonyl compounds,  $\alpha$ ,  $\beta$  unsaturated aldehydes and ketones epoxides, nitro, and oximes (with mechanism, regioselectivity, sterioselectivity and chemoselectivity).

### Unit III:

Rearrangement: Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-

Eistertreaction, Tiffeneau-Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig and Favorskii rearrangements, Dienone-phenol and Baker-Venkatraman rearrangement. Baeyer-Villiger oxidation. Neber rearrangement. Benzidine rearrangement (with mechanism, regioselectivity, chemoselectivity and sterioselectivity).

### Unit IV:

Pericyclic reaction: M.O. symmetry, Frontier orbital symmetry, FO of ethylene, 1,3-butadiene; 1,3,5- hexatriene and allyl system; Classification of pericyclic reaction, FMO, PMO and Woodward-Hoffmann correlation methods, Electrocyclic reaction - conrotatory and disrotatory motions; 4n, 4n+2 and alllyl systems, Cycloadditions- antarafacial and suprafacial additions,4n, 4n+2 systems; 2+2 addition of ketenes, 1,3- Dipolar cycloaddition Sigmatropic rearrangement— suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, 3,3 and 5,5 sigmatropic rearrangements, Claisen, Cope and Aza - Cope rearrangement.

#### Unit V:

**Photochemistry:** Photochemical Principles, Photoexcited states, Franck-Condon principles, Jablonski diagram, Intersystem crossing, singlet and triplet states, Photosensitisation, Photochemistry of carbonyl compounds (acyclic, cyclic, saturated and unsaturated systems),  $n-\pi^*,\pi-\pi^*$  transitions, Norrish type I and II reactions, Paterno-Buchi reactions, Photoreactions of ketones. Photochemistry of alkenes, cis-trans isomerisation and dimerisation.

#### SUGGESTED BOOKS:

- 1. Designing Organic Synthesis by S Warren, Wiley.
- 2. Modern Synthetic Reaction by H.O. House, WA Benzamin.
- Principles of Organic Synthesis by R. Norman & J.M. Coxon, Blackie Academic & Professional.
- 4. Advanced Organic Chemistry (Part B) by F.A. Carey & R.J. Sundberg, Plenum Press.
- Advanced Organic Chemistry by Reactions, Mechanism and Structure, Jery March. John Wiley.
- Advanced Organic Chemistry by F.A. Carey and R.J. Sundberg, Parts A & B, Plenum Press.
- 7. Stereochemistry of Organic Compounds by D. Nasipuri, New Age International.
- 8. Reaction Mechanism in Organic Chemistry by S.M. Mukherji and S.P. Singh Macmillian.
- Principles of Organic Synthesis by R.O.C Norman and J.M. Coxon, Blackie Academic & Professional.

10. S.M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, Macmillan India Ltd., New Delhi.

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## M.Sc. (Chemistry) Semester- IV

## M-Chem-402 (C) Elective Organic Chemistry of Natural products (Bio-Organic Chemistry)

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)	,	4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)	~	10 x 3=30 Marks

Unit I: Vitamins: Classification, occurrence, biological functions, structure determination and synthesis of the following: Vit. A, Vit. B<sub>1</sub>, B<sub>2</sub>, B<sub>3</sub>, B<sub>6</sub>, B<sub>7</sub>, B<sub>12</sub>, Vit. C.

(One Question from each unit)

**Unit II: Steroids and Hormones:** Occurrence, nomenclature, basic skeleton, Diels hydrocarbon, Stereochemistry, structure determination and synthesis of Cholesterol and related steroids. Cortisone and Vit. D. Structure determination and synthesis of the following: Estrogenic Hormones: Estrone, Estradiol; Gastogenic Hormones: Progesterone; Androgenic Hormones: Androsterone and Testosterone.

**Unit III: Lipids and Membranes**: Classification of lipids (Essential and Non-essential Fatty acids), Structure and function of triglycerol, glycophospholipid, lipoproteins, biological membranes, transport of cations through membranes, β-oxidation of fatty acid.

Unit IV: Enzyme Properties: Introduction, Holo enzyme (apo enzyme and coenzyme). Active site, specificity. Classification of enzymes, Allosteric enzymes. Enzyme kinetics—factors affecting rate of enzymatic reactions: enzyme concentration, substrat econcentration, pH and temperature (mention Michaelis-Menton equation), Steady state kinetics ,transition state theory, orientation and steric effects. Co-enzymes derived from vitamins, prosthetic groups; thiamine pyrophosphate, pyridoxal phosphate, NAD, NADP, NADPH, FAD, FMN, Lipoic acid and Vit. B<sub>12</sub>.

Unit V: Plant Pigment: Occurrence, nomenclature, general methods of structure determination and synthesis of Flavone, Isoflavone, Anthocyanins, Anthocyanidines, Coumarins and Chlorophyll. Biosynthesis of flavonoids.

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### SUGGESTED BOOKS:

- 1. Concise Text Book of Biochemistry by T. N. Pattabhiraman, All India Publishers.
- 2. Biochemistry by A. L. Lehninger.. al., CBS.
- 3. A Text Book of Biochemistry by A. V. S. S. Rama Rao, UBSPD.
- 4. Biochemistry by P. C. Champe and R. A. Harvey, J. B. Lippincott& Co.
- 5. Fundamentals of Biochemistry by J. L. Jain, S. Chand & Co.
- 6. Biochemistry by COSIP-ULP, Bangalore University.
- 7. Outlines of Biochemistry by Conn E. E and Stumpf P. K., John Wiley & Sons.
- 8. General Biochemistry by Weil J. H., Wiley Eastern
- 9. Biochemistry by Campbell M. K., Harcourt Brace & Co.
- 10. Principles of Biochemistry by Voet& Pratt.
- 11. Illustrated Reviews of Biochemistry by Harper.

12. Biochemistry by Stryer.

William July

## M. Sc. (Chemistry) Semester - IV M-Chem-403 (C) - Elective Organic Medicinal & Heterocyclic Chemistry

Time - 3 Hours		Full Marks: 70
Part-A		
Ten Multiple Choice Questions (Compulsory)		10 x 2=20 Marks
(Two Questions from each unit)		
Part-B		
Five Short Answer Question (Four to be Answered)		4 x 5=20 Marks
(One Question from each unit)		
Part-C		
Three Long Answer Question (Three to be Answered)		10 x 3=30 Marks
(One Question from each unit)	~	

Unit I: Drug Design: Development of new drugs, procedure followed in drug design. Structure -activity relationship (SAR), Factors affecting bioactivity, Theories of drug activity.

Unit II: Antineoplastic agents: Cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in the treatment of cancer. Synthesis of Uracil, Mustard,6-Mercaptopurine,Melphalan, Mechlorethamin; Natural products and Hormones (Excluding mechanism of drug action).

Unit III: Cardiovascular Drugs: Cardiovascular disease, direct acting arteriolar dilators, Synthesis of amyl nitrate, sorbitrate, quinidine, methyldopa, atenolol and oxyprenolol(Excluding mechanism of drug action).

**Unit IV: Antibiotics**: Structure determination and synthesis of chloramphenicol, streptomycin and penicillin, their industrial production. Anti-tubercular drugs: PAS, Isoniazid, Ethambutol, Thiosemecarbazone.

Unit V: Heterocycles: Five and six membered Heterocycles, synthesis and reactions of Benzofurans, Benzothiophenes, Benzopyrroles, Oxazole, Iso- oxazole and Imidazole. Six, seven and large membered Heterocycles, synthesis and reactions of Azepines, Oxepines, Diazepines, Diazines, Azocines, Pyrazines and Pyrimidines.

2015 WSW 278

## M.Sc. (Chemistry) Semester - IV M-Chem - 404 (C) Elective Organic Lab course

## Time - 6 Hours

Full Marks: 70

- 1. Qualitative analysis: Separation, purification, and identification of the components of mixture of organic compounds using TLC for checking the purity of the sample.
- 2. Two step synthesis of organic compounds.
- Extraction of organic compounds from natural source.
- (a) Isolation of caffeine from tea leaves
- (b) Isolation of caesin from milk
- (c) Isolation of nicotine dipicrate from tobacco
- (d) Isolation of lycopene from tomatoes
- (e) Isolation of eugenol from cloves.

OR

Separation of the compounds from mixture by paper and column chromatography

4. Identification of compounds having one or more functional groups

50 Marks

4. Note- Book

10 Marks

5. Viva-voce

10 Marks

### SUGGESTED BOOKS:

- 1. Laboratory manual of Organic Chemistry by B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi.
- 2. Practical Organic Chemistry by Mann and Saunders.
- 3. Text Book of Practical Organic Chemistry by A. I. Vogel.
- 4. Test Book of Quantitative Organic Analysis by A. I. Vogel.
- 5. A Handbook of Organic Analysis by Clarke and Hayes).
- 6. Comprehensive 'practical organic chemistry: Preparation and quantitative Analysis by V. K. Ahluwalia, R. Aggarwal, Universities Press (India).
- 7. Comprehensive practical organic chemistry: Qualitative analysis by V. K. Ahluwalia, S. Dhingra, Universities Press (India).
- 8. An advanced course in practical chemistry by A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta.
- 9. Advanced practical organic chemistry (Vol. I and II) by J. Mohan, Himalaya Publishing House.
- 10. Practical organic chemistry (Quantitative analysis) by B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi.

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