# कोल्हान विश्वविद्यालय, चाईबासा KOLHAN UNIVERSITY, CHAIBASA



रसायन शास्त्र विभाग

# University Department of Chemistry

# CBCS Syllabus Of M.Sc.

(Semester System) w.e.f Session 2017-19

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п	Core Course 4: Organic Chemistry
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Ш	Core Course 7 : Applications of Spectroscopy
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# M.Sc.

# Semester – I

# FC (Compulsory Paper)

# **Application of Computer for Chemists and Analytical Chemistry**

### Full Marks – 70

### Time :03 Hours

- 1. Eight questions are to be setatleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory).
- 3. Any Four questions out of the remaining Seven questions to be answered carrying15 marks each.

# <u>GROUP - A</u>

### I. Introduction to Computer and Computing

Basic structure and functioning of computers with a PC as an illustrative example.Memory, I/O devices.Secondary storage.Computer language.Operating systems with DOS as an example.Introduction to UNIX and WINDOWS. Data Processing, Principle of programming. Algorithms and flow-charts.

### II. Computer programming in Language

Elements of the Computer Language constant and variables and data types.Operators & Expressions, Arithmetical, Relational, Logical, Assignment, Increment and Decrement operators.Input and output statement, Branching statements such as (if – els, goto, switch) statements. Decision making and flow-charts.

### III. Programming in Chemistry

Development of small computers codes involving simple formulae in chemistry as vanderwaals equation. pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data linear simultaneous equations to solve secular equation within the Hockel theory elementary structural features such as bond lengths bond angles dihedral angles etc. of molecules extracted from a database such as Cambridge data base.

### **IV. Use of Computer Programmes**

Executionof linear regression, X-Y plot, Monte Carlo and Molecular dynamics, Programmes with data preferably from physical chemistry laboratory, Packages-MS-Word, MS-Excel, FOXPRO, MATLAB.

### **Books Suggested**

- 1. Comdex Computer course kit (XP Edition), Vikash Gupta, Dreamtech, New Delhi
- 2. Fox Pro for DOS & Windows, R.K. Taxali BPB Publication.
- 3. Programming in ANSIC, E .Balaguruswamy, Tata McGraw Hill.
- 4. Computer for Chemist, Bansal, PragatiPrakashan.

### <u>GROUP - B</u>

### I. Principles of Inorganic Analysis

Strong and Weak electrolytes, ionic equilibria, solubility and solubility product principleand their applications in qualitative inorganic analysis. Factors governing complete precipitation, partial precipitation, co-precipitation. Hydrolysis of salts.

Interfering radicals : Detection, interference and removal. Principle behind systematic qualitative inorganic analysis.

### **II. Spectrophotometric Analysis**

 $U.V-V is ible \ spectrophotometry, \ Lambart-Beer's \ Law, \ use \ of \ Spectrophotometer \ in \ the \ determination \ of :$ 

(a)Percentage composition of a mixture

- (b) Ionization constant of acid base indicator.
- (c) Composition of complex (Job's Mehtod)

### III. Use of conductometric and Potentiometric Analysis

- (a) Application of conductometric titration in the determination of :
  - (i) Dissociation constant of weak acid.
  - (ii) Basicity of weak acid.
  - (iii) Hydrolysis constant of salts derived from weak acid and strong base and vice-versa.
  - (iv) Velocity constant of saponification of ethyl acetate.
- (b) Application of potentiometric analysis in the determination of :
  - (i) Solubility and solubility product of sparingly soluble salt.
  - (ii) pH Soluble salt.
  - (iii) Instability constant of complex.

### **IV. Principles of Organic Analysis**

Detection of elements and functional groups in organic compounds, separation of compounds from the mixture, Distillation, Fractional Distillation, Distillation under reduced Pressure, Steam Distillation, Principle of Solvent extraction, Distribution Law.

Techniques of chromatographic detection and separation. Paper Chromatography, TLC, GLC.

Unit Process : Nitration, Acetylation, Sulphonation, Reduction, Oxidation, Hydrolysis and Esterification.

Estimation of (i) Phenol (ii) -OR (iii) -NH<sub>2</sub> (iv) Keto groups.

Determination of molecular weight of (i) Carboxylic Acid by silver salt method and (ii) Organic bases by platonic chloride method.

### **Books Suggested**

- 1. Skooze
- 2. Qualitative Analysis, Vogel.
- 3. Quantitative Analysis, Vogel.

### Sessional Internal Assessment (SIA) Full Marks – 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# M.Sc.

### Semester – I

### Core Course – 1

## (Inorganic Chemistry)

### Full Marks - 70

**Time :03 Hours** 

- 1. Eight questions are to be set at least one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered carrying15 marks each.

### I. Stereochemistry and Bonding in Main Group Compounds

VSEPR theory, Walsh diagrams (tri-atomic molecules type AH2),  $d\pi$ -p $\pi$  bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules, Atomic Inversion, Berry Pseudorotation.

### II. Metal – Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

### **III. Reaction Mechanism of Transition Metal Complexes**

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories.Kinetics of octahedral substitution.Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, reactions without metal ligand bond cleavage. Substitution reaction in square planer complexes, the trans effect, mechanism of substitution reactions.

### **IV. Metal – Ligand Bonding**

Limitations of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, Jahn-Teller effect,  $\pi$  – *bonding* and molecular orbital theory.

### V. Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, correlation, Orgel and Tanbe-Sugano diagrams for transition metal complexes  $(d^1 - d^2 \text{ states})$ , calculations of Dq, B and  $\beta$  parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

### VI. Metal $\pi$ Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphines as ligand.

### **Books Suggested**

- 1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson. John Wiley.
- 2. Inorganic Chemistry, J.E. Huhey, Harpes& Row.
- 3. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamom.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Magneto Chemistry, R.L. Cariin, Springer Vertag.
- 6. Comprehensive Coordination Chemistry, Q. Wilkinson, R.D. Gillars & J.A. McCleverty, Perganom.
- 7. UGC Advanced Inorganic Chemistry, S.K. Agarwal&KimatiLal.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# M.Sc.

# Semester – I

# Core Course - 2

# (Physical Chemistry)

### Full Marks :70

Time : 03 Hours

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered carrying 15 marks each.

### I. Quantum Chemistry

### A. Introduction to Exact Quantum Mechanical Results

The Schrodinger question and the postulates of quantum mechanics.Discussion of solutions of the Schrodinger equation to some model systems viz..., particle in a box, the harmonic oscillator, the rigid rotor.The hydrogen atom.

### **B.** Electronic Structure of Atoms

Electronic configuration, Russell – Saunders terms and coupling schemes, Slater – Condon parameters, term, separation, energies of the  $p^n$  configuration, term separation energies for the  $d^n$  configuration, magnetic effects : spin – orbit coupling and Zeeman splitting, introduction to the methods of self – consistent field. The virial theorem.

### C. Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations, Application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended huckel theory.

### II. Thermodynamics

### A. Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial moarproperties ; partial molar free energy, partial molar heat content of fugacity. Non-ideal systems : Excess functions for non-ideal solution. Activity, activity coefficient.

### **B.** Statistics Thermodynamics

Concepts of distribution, Thermodynamic probability and probable distribution.Ensemble averaging postulates of ensemble averaging.Canonical, grand Canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition function – translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions.

### III. Chemistry Dynamics

Method of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory ; ionic reaction, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, kinetic salt effects, and thermodynamic control of reaction, treatment of unimolecular reactions.

### **IV. Surface Chemistry**

### A. Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation)surface films on liquids (Electro – kinetic phenomenon), catalytic activity at surfaces.

### **B.** Macromolecules

Polymer – definition, types of Polymers, electrically conducting fire resistant liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass.Number and mass average molecular mass.Determination (osmometry, viscometer, diffusion and light scattering method sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

### V. Electrochemistry

Electrochemistry of solutions.Debye-Huckel-Onsager treatment and its extension ion solvent interaction.Deby-Huckel-Jerum mode.Thermodynamics of electrified interface equations. Derivation of electro-capillarity, lippmann equations. (surface excess), methods of determination.

Debye – Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

### **Books Suggested**

- 1. Physical Chemistry, P.W. Atkins. ELBS.
- 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- 4. Coulson's Valance, R. Me Weeny, ELBS.
- 5. Chemical kinetics, K.J. Laidler, Megraw-Hill.
- 6. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J. Kuriacose, Mcmillan.
- 7. Micelles, Theoriticals and Applied Aspects, V. Morai, PlenLM
- 8. Modern Electrochemistry Vol.-II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
- 9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
- 10. Advanced Physical Chemistry, Gurtu&Gurtu, PragatiPrakashan.
- 11. Quantum Chemistry, R.K. Prasad
- 12. Advanced Physical Chemistry, D.N. Bajpai.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# M.Sc.

Semester – I

Full Marks – 100

Core Course Practical-3

Time: 06 Hours

### <u>Group – A</u> (Inorganic Chemistry Practical)

One experiment from the following should be set.

- 1. Cent per cent quantitative Analysis of the following (i) dolomite (ii) cement (iii) pyrolusite
- **2.** Quantitative analysis of (i) Haematite by  $KMnO_4$  and  $K_2Cr_2O_7$  (ii) common solder and (iii) brass
- **3.** Estimation of the following :
  - (a) Magnesium by E.D.T.A. methods (volumetrically)
  - (b) Zinc by potassium ferrocyanide (volumetrically)
  - (c) Nickel by dimethylglyoxime (gravimetrically)
  - (d) Mangancese in steel by sodium bismuthate method.
- **4.** Preparation of the following metal complexes & their studies by IR, electronic spectra, mossabuar, ESR & magnetic susceptibility measurement.
  - (a) Hexaminecobltic chloride.
  - (b) Sodium nitroprusside.
  - (c) Prussian blue
  - (d) Potassium trioxalatoferrate (III)  $K_3[Fe(C_2O_4)_3]$
  - (e) Nickel Dimethylglyoxime. Ni(dimg)<sub>2</sub>

### <u>Group – B</u>

### (Computer Practical)

One experiment from the following should be set.

- 1. Familiarity and use of scientific package such as Scientific Work Place (Scientific Word Processor), Spreadsheets, Data-base.
- 2. Programming examples in C to handle the following problems in Chemistry :
- i. Polynomial equation and polynomial equation fitting.
- ii. Matrix inversion and diagonalization.
- iii. Empirical/molecular formula from elemental analysis.
- iv. Molecular formula from mass spectroscopy.
- v. pH of a weak acid-base titration.
- vi. Potentiometric end point-titration.
- vii. Stimulation of Maxwell-Boltzmann distrinution.
- viii. R.M.S. Velocity and kinetic energy of a gaseous particle in 3-degree of freedom.
- ix. Half-life period of nuclear decay.

Experiments- 40 + 40 Marks

Viva-Voice -5 + 5 Marks

Notebook- 5 + 5 Marks

# Chemistry M.Sc Semester – II

### Core Course – 4

# (Organic Chemistry)

#### Full Marks - 70

**Time :03 Hours** 

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### I. Nature of Bonding in organic Molecules and reaction mechanism

Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbon, Huckel's rule, energy level of  $\pi$  molecular orbitals, annulenes, anti-aromaticity,  $\Psi$  aromaticity, bomo-aromaticity, PMO approach.

Bonds weaker then covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

### **RectionMechanism : Structure and Reactivity**

Type of mechanisms, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle.Potential energy diagrams, transition states and intermediates, methods of determining mechanisms.

### **II.** Sterochemistry

Conformational analysis of cycloalkanes, decalins, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis.Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.

### III. Aliphatic and aromatic Nucleophilic Substitution

The  $S_N^{\ 2}$ ,  $S_N^{\ 1}$ , mixed  $S_N^{\ 1}$  and  $S_N^{\ 2}$  and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S<sub>N</sub><sup>1</sup>mechanism.

Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon.

### IV. Aliphatic and aromatic Electrophilic substitution

Bimolecular mechanisms  $-S_E^2$  and  $S_E^1$  mechanism, electrophilic substitution accompanied by double bond shifts. Effects of substrates, leaving group and the solvent polarity on the reactivity. The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophics. Diazonium coupling, Gattermann-Koch reaction.

### **Aromatic Nucleophilic substitution**

The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms.Reactivity-effect of substrate structure, leaving group and attacking nucleophile.The von – Richter, Sommelet Hauser, and Smiles rearrangement.

### V. Addition to Carbon-Carbon Multiple Bonds and Carbon Hetero Multiple Bonds

Mechanistic and steriochemical aspects of addition reactions involving electrophiles.Nucleophiles and free radicals, region – and chemoselectivity, orientation and reactivity.Addition to cyclopropane ring.Hydrozenation of aromatic rings.Hydrobaration.Michael reaction.Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc and organilithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction.

Mechanism of condensation reaction involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Hydrolysis of esters and amides, ammonolysis of esters.

### VI. Elimination Reaction

The E2, E1 and E1cB mechanisms and their spectrum.Orientation of the double bond.Reactivity-effect of substrate structures, attacking base, the leaving group and the medium.

Mechanism and orientation in pyrolytic elimination.

### VII. Pericyclic Reactivity

Molecular orbital symmetry, Frontier orbital's of ethylene, 1.3-butadiene 1, 3, 5-hexatriene and anyl system. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction – conrotatory and disrotatory motions, 4n, 4n + 2 and allyl systems Cycloaddition– antarafacial additions, 4n and 4n+2 systems, 2 + 2 addition of ketenes 1, 3 dipolar cycloadditions and chelotropic reaction.

### **Book Suggested**

- 1. Advanced Organic Chemistry Reaction, Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
- 6. Modern Organic Reaction, H.O. House, Benjamin.
- 7. Principles of Organic Synthesis, R.O.C. Norman & J.M. Coxon, Blackle Academic & Professional.
- 8. Pericycllc Reaction, S.M. Mukherji, Macmillan, India.
- 9. Reaction Mechanism in Organic Chemistry, S.M. Mukharji and S.P. Singh, Macmillan.
- 10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 11. Stereochemistry of Organic Compounds. P.S. Kalsi, New Age International.
- 12. Mechanism of Organic reactions, K.S. Mukherjee, Books and Allied (P) Ltd. Kolkata.
- 13. Photo chemistry and Pericyclic Reactions, Jagadamba Singh and Jaya Singh, New Age International Publishers.

### Sessional Internal Assessment (S/A) Full Marks – 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# M.Sc.

# Semester – II

# Core Course – 5

### **Group Theory and Spectroscopy**

### Full Marks - 70

### Time :03 Hours

- 1. Eight questions are to be set at least one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### Group Theory, Spectroscopy and Diffraction method

### I. Symmetry and Group Theory in Chemistry

Symmetry and elements and symmetry operation, definitions of group, subgroup, relation between order of a finite group and its subgroup.Conjugacy relation and classes.Point symmetry group.Schonflies symbols. Representation of groups by matrices (Representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked out explicitly) Character of a Representation. The great orthogonality theorem (without proof) and its importance. Character tables their use; spectroscopy.

### II. Vibrational Spectroscopy

### A. Infrared Spectroscopy

Review of linear harmonic oscillator, Vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, Vibration-rotation Spectroscopy, P, Q, R, branches. Breakdown of Oppenheimer approximation; Vibrations of polyatomic molecules. Selection rules, normal modes of Vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal – ligand vibrations, normal co-ordinate analysis.

### B. Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational rotational Raman spectra, selection rules mutual exclusion principle. Resonance Raman Spectroscopy, Coherent Anti stokes Raman Spectroscopy (CARS).

### III. Electronic Spectroscopy

### A. Atomic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling spectra of hydrogen atom and alkali metal atoms.

### **B.** Molecular Spectroscopy

Energy levels, molecular orbitals, vibronic transition, vibrational progressions and geometry of the excited states, Franck – Condon Principle, electronic spectra of polyatomic molecules.Emission spectra; radiative and non-radiative decay, internal conversion, metal complexes, charge – transfer spectra.

### IV. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, Nuclear resonance, saturation shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin-spin interaction, factors influencing coupling constant 'J' Classification (ABX, AMX, ABC,  $A_2B_2$  etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton – <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P. FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

### V. Electron Spin Resonance Spectroscopy

Basic principle, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship measurement techniques, applications.

### VI. X-ray Diffractions

Bragg condition, miller indices, Laue method, Bragg method, Debye – Scherer method of X-ray structural analysis of crystals, index reflections identification of unit cells from systematic absences in diffractions pattern.Structures of simple lattices and X-ray intensities, structure factor and its relation analysis, absolute configuration of molecules, Ramchandran diagram.

### **Book Suggested**

- 1. Modern Spectroscopy, J.M. Hollas, John Wiley.
- 2. Applied electron Spectroscopy for Chemical Analysis, Ed. H. Windawi and F.L. Ho. Willy Interscience.
- 3. NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
- 4. Physical method in Chemistry, R.S. Drago, Saunders College.
- 5. Chemical Application of Group Theory, F.A. Cotton.
- 6. Introduction to Molecular Spectroscopy, Q.M. Barrow, McCraw Hill.
- 7. Basic Principle of Spectroscopy, R.Chang, McOraw Hill.
- 8. Theory and Application of UV Spectroscopy, H.H. Faffe and M. Orchin, IBH-Oxford.
- 9. Introduction of Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
- 10. Introduction of Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Raw.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

Pass Marks = 17

08 Hrs.

12 Hrs.

12 Hrs.

# M.Sc.

### Semester – II

### Core Course – 6 (Practical)

Full Marks - 100

Time :06 Hours

### Group – A

### (Organic Chemistry Practical)

One experimentfrom the following should be set.

### I. Organic Qualitative Analysis

Identification of organic compounds containnot more than two functional; groups using chemical analysis.

### II. Preparation of organic compounds using methods not involving more than two steps :

- (i) Preparation of Methyl Orange
- (ii) Preparation of 2, 4, 6 Tribromo phenol from Aniline
- (iii) Preparation of p-Nitro aniline from Acetanilide
- (iv) Preparation of Sulphanilic acid from Aniline

### III. Estimation of

- (i) Glucose
- (ii) Carbonyl group using 2, 4 Dinitrophenyl hydrazine (DNP)

### Group – B (Physical Chemistry Practical)

One experiment from the following should be set.

### I. Measurement of density of gases and vapours

Victor meyer's method determination of molecular weight of acetone, Chaloroform, benzene, (mixture).

### II. Determination of molecular weight of substances

Backmann's freezing point method

#### III. Viscosity of Liquids and Solution by Ostwald tube.

Determination of percentage composition of a mixture of two liquids.

### **IV. Surface Tension of Liquids and Solutions**

- (a) Determination of surface tension of the given liquid by drop number method.
- (b) Determination of Parachor

### V. Thermochemistry

- (a) Determination of water equivalent of a calorimetry
- (b) Determination of Heat of Neutralization of :
  - (i) Strong acid and strong Base (HCl and NaOH)
  - (ii) Weak acid and strong Base (NaOH and CH<sub>3</sub>COOH)

### **VI. Order of Reaction**

- (a) Determination of rate constant of hydrolysis of an ester with an acid (Methylacetate and HCl)
- (b) Determination of the rate constant of saponifaction of ethylacetate by NaOH.

### VII. Partition Co-efficient

Determination of partition coefficient of :

- (i) Benzoic acid between water and Benzene
- (ii) Iodine between water and Carbon tetrachloride.

### **Experiments**

Group A – 40 Marks

Group B – 40 Marks

Notebook -5 + 5 Marks

Viva-voce -5 + 5 Marks

# Chemistry M.Sc.

### Semester – III

### Core Course – 7

# **Application of Spectroscopy**

### Full Marks - 70

### **Time :03 Hours**

1. Eight questions are to be set atleast one question from each chapter.

- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### **Inorganic Chemistry**

### I. Vibrational Spectroscopy

Symmetry and shapes of AB2, Abs, AB4, Abs and ABc, mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

### II. Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH<sub>4</sub>, F<sub>2</sub> and [BH<sub>3</sub>].

### III. Nuclear Magnetic Resonance of Paramagnetic Substances in Solution

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis on <sup>195</sup>Pt and <sup>119</sup>Sn NMR.

### IV. Mossbauer Spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of  $Fe^{+2}$  and  $Fe^{+3}$  compounds including those of intermediate spin. (2)  $Sn^{+2}$  and  $Sn^{+4}$  compounds nature of M-L bond, co-ordination number, structure and (3) detection of oxidation and in equivalent MB atoms.

### **Organic Chemistry**

### I. Ultraviolet and Visible Spectroscopy

Various electronic transitions (185-800 nm), Beer – Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclie compounds.

### II. Infrared Spectroscopy

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbony compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyi compounds). Effect of hydrogen bonding and solvent effect on vibrations frequencies, overtones, combination bands and Fermi resonance, FT, IR, IR of gaseous, solids and polymeric materials.

### III. Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phensols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique.

### **Carbon 13 NMR Spectroscopy**

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and Carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, NIEPT.

### IV. Mass Spectrometry

Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

### **Book Suggested**

- 1. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- 2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
- 3. Infrared and Raman Spectra : Inorganic and Co-ordination Compounds, K. Nakamoto, Wiley.
- 4. Progress in Inorganic Chemistry Vol. 8, ed, F.A. Cotton, Vol. 15, ed, S.J. Lipard, Wiley.
- 5. Transition Metal Chemistry eA.R.L. Carlin Voi. S. Dekker.
- 6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.

### Sessional Internal Assessment (SIA) Full Marks – 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# M.Sc.

### Semester – III

### Core Course – 8

# (Bio Inorganic and Bio Organic)

### Full Marks - 70

### **Time :03 Hours**

- 1. Eight questions are to be set in which.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory).
- 3. Three questions from Group A and four questions from Group B are to be set out of which four questions are to be answered selecting at least one question from each group. Each question will carry 15 marks.

### Group – A

### (Bio-inorganic)

### I. Metal Ions in Biological Systems

Essential and trace metals.

Na' / K' Pump

Role of metals ions in biological processes.

### II. Bioenergetics and ATP Cycle

DNA polymerization, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water, Model system.

### III. Transport and Storage of Dioxygen

Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanics and hemerythrin, model synthetic complexes of iron, cobalt and copper.

### IV. Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes – cytochromes and ion-sulphur proteins, synthetic models.

### Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model system.

# Group – B

### (Bio-organic)

### I. Enzymes and Mechanism of Enzyme Action

Basic considerations, Proximity effects and Molecular adaption.

### Enzymes

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshtand's induced fit hypothesis, concept and identification of active site by the use of inhibitors. Affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweave-Burk plots. Reversible and irreversible Inhibition.

### Mechanism of Enzyme Action

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion.Examples of some typical enzyme mechanisms for chymotrypsin, lysozyme and carboxypeptidase A.

### II. Kinds of Reactions Catalysed by Enzymes

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reaction. Enolic intermediates in isomerization reactions. P-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

### III. Co-Enzyme Chemistry

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD, NADI, FMN, FAD, Lipole acid, vitamin B12, Mechanisms of reactions catalyzed by the above cofactors.

### IV. Biotechnological Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in feed and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

### **Book Suggested**

- 1. Principles of Bio-inorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 2. Bio-inorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books
- 3. Inorganic Bio-Chemistry vols A and II, Ed. G.I..... Eichhorn, Elsevier.
- 4. Progress in Inorganic Chemistry, Vols 18 and 3S Ed. J.J. Lippard, Wiley.
- 5. Bio-organic Chemistry : A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
- 6. Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 7. Enzyme Chemistry : Impact and Application, Ed. Collin J. Suckling, Chapma and Hail.
- 8. Enzyme Mechanisms Ed. M.I Page and A. Villiams, Royal Society of Chemistry.
- 9. Fundamentals of Enzymology, N.C. Price and L. Slovens, Oxford University Press.
- 10. Immobilized Enzymes : An Introduction and Applications in Biotechnology, Michael O. Trevan, John Wiley.
- 11. Enzymatic Reaction Mechanisms, C. Walsh, W.H. Freeman.
- 12. Enzyme structure and Mechanism, A. Fersht, W.H. Freeman.
- 13. Bio-Chemistry : The Chemical Reactions of Living Cells, D.E. MeUler. Academic Press.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

### M.Sc.

### Semester – III

### EC 2

# **Inorganic Chemistry (Special)**

### Full Marks - 70

#### **Time :03 Hours**

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### I. Alkyls and Aryls of Transition Elements

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

### II. Compounds of Transition Metal – Carbon Multiple Bonds

Alkylidenes, alkyledynes, low valentcarbenes and carfynes-synthesis, nature of bond, structural characteristics, nucleophile and electrophilic reactions on the ligands, role of organic synthesis.

### III. Transition metal $\pi$ Complexes

Transition metal  $\pi$  Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, areneandtrienyl complexes, preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

### **IV. Homogeneous Catalysis**

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta Polymerization of Olefins, catalytic reaction involving carbon monoxide such as hydrofomylation of olefin (oxo reaction), oxopalladation reactions activation of C-H bond.

### V. Fluxional Organometallic Compounds

Fluxionality and dynamic equilibrium in compounds such as  $\eta$ -olefine,  $\eta$ -allyl and dienyl complexes.

### **Book Suggested**

- 1. Principles and Application of Organochemistry Metal Chemistry, J.P. Collman, L.S. Hegsdus. J.R. Norton and R.G. Pinke, University Science Books.
- 2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
- 3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
- 4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# Chemistry M.Sc. Semester – III

### EC 2

# **Organic Chemistry**(**Special**)

### Full Marks - 70

**Time :03 Hours** 

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### I. Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, Isoprene rule.

Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules :Citral,  $\alpha$ -Terpineol, $\alpha$ -Pinene.

### II. Alkaloids

Definition, nomenclature and Physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, Stereochemistry, synthesis and biosynthesis of the following : Atropine, Quinine and Morphine, Narcotine.

### **III.** Steroids

Occurrence, nomenclature, basic skeletion, Diel's Hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Estrone, Progestrone, Biosynthesis of steroids.

### IV. Concept of Molecular Orbital (MO) and Valence Bond (VB) Theory

Quantitative MO Theory - Hiickel Molecular Orbital (HMO) method applied to ethane, allyl and butadiene. Qualitative MO theory-ionisation potential, Electron affinities.MO energy levels.Orbital symmetry. Orbital interaction diagrams, MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group.

Valence Bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory, Reaction profiles, Potential energy diagrams. Curve-crossing model-nature of activation harrier in chemical reactions.

### V. Principles of Reactivity

Mechanistic significance of entropy, enthalpy and Gibbs free energy, Arrhenius equation.Transition state theory.Uses of activation parameters, Hammond's postulate.Bell-Evans-Polanyl principle.Potential energy surface model, Marcus theory of electron transfer.Reactivity and Selectivity principles.

### VI. Structural Effects on Reactivity

Linear Free Energy Relationship (LFER), The Hammett equation, Substituent constants, theories of substituent effects, Interpretation of  $\sigma$ -values. Reaction constant p. Derivations from Hammett equation.Dual-parameter correlation, inductive substituent constant, The Taft model. $\sigma_1$  and  $\sigma_R$  scales.

### VII. Solvation and Solvation Effects

Qualitative understanding of solvent – solute effects on reactivity. Thermodynamic measure of solvation. Effects of salvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties, solvent sensitive reaction rates, spectroscopic properties and scales for specific salvation. Use of salvation scales in mechanistic studies. Solvent effects from the curve-crossing model.

#### Sessional Internal Assessment (S/A) Full Marks – 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# Chemistry M.Sc. Semester – III EC 2 Physical Chemistry(Special)

### Full Marks - 70

### Time :03 Hours

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc. 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.
- I. Diffraction of X-rays by crystals-Debye Scherrer method, indexing powder pattern for cubic and tetragonal crystals, rotating crystal method, Fourier transform and reciprocal lattices, Bragg equation in reciprocal. Lattice, neutron diffraction.
- **II. Metallic bonds** free electron theory, bond theory, Fermi level, Brillouin zone, wave function for electrons in solids, metallic conductors, insulator, semiconductors (intrinsic & extrinsic), properties of junctions.
- **III. Super conductivity** meissener effect, microscopic theory of super conductivity, conventional organic and high temp, super conductors, fullerenes, applications of superconductors transformation of order disorder transitions, martensitic transition, polymorphic, transformation.
- **IV.** Specific heat of solids classical theory, quantum theory of specific heats einstent and debye theories, characteristic temp. and its calculation, T-law solid state reaction, laws governing nucleation. Homogeneous and heterogenous nucleation, thermodynamic barrier.
- V. Polymer solution thermodynamics of polymer solution, molar mass and molar mass distribution, methods of measuring molar masses, micelle formation and hydrophobic interaction. Electrically conducting polymers, electrochemical polymerization, band structures of polymers mechanism of conduction in polymers, doping of polymers, application of conduction polymers.
- **VI.** Polymers liquid crystals nematic, cholesteric and smectic phases, liquid crastoline order of the main chain and of the side groups in polymers, synthesis and properties of polymers liquid crystals, liquid crystalline order in biological material.
- **VII.** Surface chemistry surface films, BET isotherm for, multilayers & its derivation, kinetics of surface processes, unimolecular and bimolecular surface reaction, electrocapillarity, electro kinetic effect, statistical mechanics of adsorption.

### **Book Suggested**

- 1. Crystallography Philips
- 2. Solid State Chemistry Garner (Butterworth; London)
- 3. Solid State Chemistry D.K. Chakraborty (New Age Publication)
- 4. Solid State Chemistry N.B Hannay (Prentice Hall, New Jersey)
- 5. Physical Chemistry Waller J. Moore
- 6. Physical Chemistry P.W. Atkins
- 7. Principle of polymer Chemistry Cornell, P.J. Flory (University Press)
- 8. Handbook of Conducting polymers Vol I & II, T.A. Skolhia.

### Sessional Internal Assessment (S/A) Full Marks – 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

M.Sc.

### Semester - III

### EC 3 (Practical)

# **Inorganic Chemistry (Special)**

### Full Marks - 100

**Time :06 Hours** 

### Two questions are to be set

### I. Quantitative Analysis

- (i) Analysis of alloys (brass type metal, solder, gun metal) Cement, Steel Using conventional chemical analysis / and physical techniques (if possible). (Preferably one alloy and cement analysis may be carried out).
- (ii) Analysis of two cation-system using complexones.
- (iii) Colorimetric estimation of cation/anions.
- **II.** Separation Techniques
  - (i) Ion exchange : Separation of inorganic cations/anions (2 or 3 components).
  - (ii) Chromatographic Separation.
    - (a) Cd Zn (b) Zn Mg
- III. Preparation of inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods.
  - (i) Preparation of Cobalt (III) complexes
    - (a)  $[Co(NH_3)_5Cl]Cl_2$
    - (b)  $[Co(NH_3)_5NO_2]Cl_2$
    - (c) [Co(NH<sub>3</sub>)<sub>5</sub>ONC]Cl<sub>2</sub>

Experiments - 80Marks

Viva-Voice -10 Marks

Notebook –10 Marks

M.Sc.

### Semester – III

# EC 3 (Practical)

# **Organic Chemistry (Special)**

### Full Marks - 100

**Time :06 Hours** 

### Two questions are to be set

### I. Organic Synthesis and Extraction of Organic Compounds from Natural Sources

The students are expected to carry out 6 to 8 organic preparation (usually involving not more than two steps). Some of the illustrative experiments are listed below:

- Extraction of caffeine from tea leaves (Ref. Experimental Organic Chemistry H Dupon Durst. George W. Gokel, p.464 MnGraw Hall Book Co., New York). Students should be asked to purify the crude sample, check the purity on TLC single spot and/or get the pmr scanned and interpret. (Three methyl singles and 1 methine singlet).
- 2. Isolation of casein from milk (Try som typical colour reactions of proteins).
- 3. Isolation of lactose from milk (check purity of sugar by TLC and PC and calculated Rf value).
- 4. Isolation of nicotine dipicrate form tobacco.
- Synthesis of 3-nitrobenzoic acid from benzoic acid. (Ref.: ibid, p.246-247 and 443-448). Aim to demonstrate the process of metanitration, esterification and saponification of ester. Make a comparative study of IR and PMR spectra of bezoic acid, methyl benzoate, methyl nitrobenzoate, if possible.
- 6. Preparation of Indigo from anthranilic acid.
- Cannizzaro reaction of 4-chlorobenzaldehehyde (Ref.: ibid. p. 397-400). Aim to demonstrated technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer. Make a comparative study of IR and PMR spectra of 4-Chlorobenzyl alcohol, fi possible.
- 8. Synthesis of benzanilide from benzene (Ref.: ibid. p. 775, 812)
  Aim to carry out Friedal Crafts Acylation (anhydroup conditions) and Beckmann rearrangement.
  Make a comparative study of IR and PMR spectra of benzene, benzophenone, benzophenoneoxime and benzanilide (N-H stretching vibration typical of a secondary amide) if possible.
- **II.** Characterization of organic compounds. The student is expected to carry out analysis of components of binary organic mixture (liquid-liquid, liquid-solid, solid-solid). Using chemical analysis and IR and PMR data. The students should also to check the purity of the separated components on TLC plates.
- Experiments 80 Marks

Viva-Voice - 10 Marks

Notebook - 10 Marks

# Chemistry M.Sc. Semester – III EC 3 (Practical) Physical Chemistry (Special)

Full Marks - 100

**Time :06 Hours** 

### Two questions are to be set

### I. Conductometry

- (a) To determine the solubility and solubility product of a sparingly soluble salt.
- (b) To verify Onsager equation for a uni-univalent electrolyte in aqueous solution.
- (c) To titrate a mixture of HCI, CH<sub>3</sub>COOH and CuSO<sub>4</sub> with NaOH.
- (d) To determine the rate constant of saponification of an ester by NaOH.

### **II.** Potentionmetry

- (a) To determine the solubility and solubility product of AgCI in water.
- (b) To determine the  $E^{\circ}$  of  $Zn/Zn^{2+}$ ,  $Cu/Cu^{2+}$  Electrodes.
- (c) To determine the basicity of polybasic acid and its dissociation constant.
- (d) To investigate the complex formed between  $CuSo_4$  and  $NH_3$ .

### **III.** Polarimerty

- (a) Determination of specific rotation of sucrose.
- (b) Study of inversion of cane sugar in acid medium.

### **IV. Refractometry**

- (a) To verify mixture law of refraction.
- (b) To determine the composition of an unknown solution.

### V. Cryoscopy

- (a) To determine to activity of a non-electrolyte by freezing point method.
- (b) To determine the mean activity co-efficient of KCI by freezing point method.

### VI. Conductivity

- (a) Determination of cell Constant
- (b) Determination of equivalent conductivity of weak acid (acetic and succinic acid) at several concentrations and calculation of the dissociation constant of the acid.
- (c) Determination of the basicity of an acid (Citric acid and Oxalic acid)
- (d) Titration of :
  - (i) Strong acid and Strong Base (HCl and NaOH)
  - (ii) Weak and Strong Base (CH<sub>3</sub>COOH and NaOH)

### VII. E.M.F.

- (a) Determination of Single electrode potential of Cu/Cu<sup>2+</sup>
- (b) Determination of e.m.f of conc. cell
- (c) Potentiometric Titration of acid-base
- Experiments 80 Marks

### Viva-Voice – 10 Marks

Notebook - 10 Marks

# Semester – IV

# Core Course – 9

### (Environmental Science and Green Chemsitry)

### Full Marks - 70

#### Time :03 Hours

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

### I. Environment

Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, Biogeochemical cycles of C, N, P, S and O. bio distribution of elements.

### II. Hydrosphere

Chemicals compositions of water bodies-lakes, streams, rivers, and wet lands etc. hydrological cycle, Aquatic Pollution – inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand (BOD), Solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganism.Water quality standards, Analytical methods for measuring BOD, DO, COD, F, Oils, Metals (As, Cd, Cr, Hg, Pb, Se etc.). Residual chloride and chlorine demand. Purification and treatment water.

### III. Atmosphere

Chemical composition of atmosphere-particles, ions and radical and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorocarbons (CFC's). Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

### **IV.** Industrial Pollution

Cement, Sugar, Distillery, Paper and Pulp, thermal power plants, nuclear power plants, metallurgy, polymer, drugs etc. Radionuclide analysis, Disposal of wastes and their management.

### V. Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles and decomposition. Better industrial process, Bhopal Gas tragedy, Chernobyle, Three miles Island, Sewozo, and Minamatadiasters.

### VI. Green Chemistry : Definition and Objective

The twelve principles of Green Chemistry, atom economy in chemical synthesis, important technique employed in practice of Green Chemistry, Application of microwave irradiation and ultrasound in chemical reactions.Use of renewable raw materials and biosynthesis, organic waste management, use of safer reagents and green solvents and green catalysts.

### VII. Green Chemistry : Real Applications

Replacement of CFC and hydrocarbon blowing agents with environmental friendly blowing agent  $CO_2$  in the production of polystyrene. Replacement of Ozone depleating and Smog producing solvents by surfactant assisted liquid or supercritical carbon dioxide for cleaning in manufacture of ICs and Computer chips.

### **Books Suggested**

- 1. Environmental Chemistry and Green Chemistry, Asin Kr Das, Books and Allied (P) Ltd. Kolkata.
- 2. Environmental Chemistry, H. Kaur, PragatiPrakashan.
- 3. Environmental Chemistry, S.F. Manahan, Lewis Publishers
- 4. Environmental Chemistry, A.K. Dey, Wiley Easlem.
- 5. Environmental Chemistry, C. Baird, W.H. Freeman.

### Sessional Internal Assessment (SIA) Full Marks – 30 Marks

A – Internal written Examination – 20 Marks (1 Hr)

- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# Chemistry M.Sc Semester – IV EC 4 (Inorganic ChemistrySpecial)

#### Full Marks – 70

**Time :03 Hours** 

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

#### I. Metal storage transport and Biomineralization

Ferritin, Transferring and Siderophores.

#### II. Calcium in biology

Calcium in living cells, transport and regulation, molecular aspects of intramolecular process, extracellular binding proteins

#### III. Metallelloenzymes

Zinc emzymes – corboxypeptidase and carbonic anhydrase. Iron enzymes – catalase peroxidase and cytochrome P-450. Copper enzymes – super oxide dismutase.

Molybdenum oxatransferase enzymes xanthine oxidase.Coenzyme vitamin B<sub>12</sub>.

#### IV. Metal-Nucleic Acid Interactions

Metal ions and metal complex interactions, meal complex - nucleic acid.

#### V. Metals in Medicine

Metal deficiency and disease toxic effect of metals, metals used for diagnosis and chemotherapy eith particular reference to anticancer drugs.

### VI. Supramolecular Chemistry

Concept and language

- (a) Molecular recognition Molecular receptors for different type of molecular including arisonic substrates design and synthesis of coreceptor molecules and multiple recognition.
- (b) Supramolecular reactivity and catalysis.
- (c) Transport processes and carrier design.
- (d) Supramolecular devices, supramolecular photochemistry, supramoleular electronic, ionic and switching devices.

Some example of self assembly in supramolecular chemistry.

#### Book Suggested

- 1. Principles of Bioinorganic Chemistry, S.J. Lippard, J.M. Berg, University Science Books.
- 2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- 3. Inorganic Biochemistry vol I and II, Ed. O.L. Eichhom, Elsevier.
- 4. Progress in Inorganic Chemistry, Vols 18 and 38 Ed. J.J. Lippard, Wiley.
- 5. Supramolecular Chemistry, J.M. Lehn, VCH.

#### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

A – Internal written Examination – 20 Marks (1 Hr)

- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# Chemistry M.Sc. Semester – IV EC 4 (Organic ChemistrySpecial)

#### Full Marks - 70

**Time :03 Hours** 

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

#### I. Six – membered Heterocycles with one heteroatom

Synthesis and reaction of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridines.

Synthesis and reaction of quinolizinium and their benzopyrilium salts, coumarins and chromones.

Six – membered heterocycles with Two or More Heteroatoms

Synthesis and reaction of diazines, tetrazines and thiazines.

II. Structure determination and synthesis of Vit. A, B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub>, Vit. C and Vit. D.

### III. Acids, Based, Electrophiles, Nucleophiles and Catalysis

Acid, base dissociation, electronic and structural effects, acidity and basicity, acidity functions and their applications, hard and soft acids and bases,nuclcophilicity,acid base catalysis, specific and general catalysis. Bronsted catalysis,nucleophilic and electrophilic, catalysis.

#### **IV. Steric and conformational properties**

Various type of steric strain and their influence on reactivity steric acceleration molecular measurements of steric effects upen rates. Steric LFER.Conformational barrier to bond rotation spectroscopic detection of individual.Conformers acyclic and mono cyclic system rotation around partial double bonds WinsteinHolness and Curtin. Hammett principle.

### V. Nueleophilic and electrothilic reactivity

Structural and electronic effects on  $SN_1$  and  $SN_2$  reactivity solvent effect kinetic isotope effects inter molecular assistance electron transfer nature of  $SN_2$  reaction. Nucleophilicity and  $SN_2$  reaction based on curve, crossing model.Relationship between polar and electron transfer reaction. $S_{RN}1$ mechanism.Electrophilic reactivity, general mechanism.Kinetic of  $S_E2$  – Ar reaction. Structural effects on rates and selectivity, Curve – crossing approach to electrophilic reactivity.

### VI. Supramolecular Chemistry

Properties of covalent bonds – bond length, inter – bond angles, force contant, bond and molecular dipole moment. Molecular and bond polarizability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effect, electrostatic, induction, dispersion and resonance energy, magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects, Hydrogen bond. Principle of molecular association and organization as exemplified in biologicalmacromolecules like enzymes, nucleic acids.

### **Books Suggested**

- 1. Molecular mechanics, U. Burkertand, N.L. Allinger, ACS Monograph 177, 1982.
- 2. Organic Chemists' book of OrbMals. L. Salem and W.L. Jorgensen, Academic press.
- 3. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
- 4. Introduction theoretical Organic Chemistry and molecular. Modeling, W.B. Smith. VCH. Weinheim.
- 5. Physical Organic Chemistry, N.S. Issacs, ELBS/Longranan.
- 6. Supramolecular Chemistry; Concepts and perspectives, J.M. Lehn, VCH.
- 7. The Physical basis of Organic Chemistry, H. Maskill, Oxford University press.
- 8. Heterocyclic Chemistry Vol. 1-3, R.R. Supta, M. Kumar and V. Gupta, Springer verlag.
- 9. The Chemistry of heterocycles, T. Eicher and S. Hauptmann, Theime.
- 10. Heterocyclic Chmistry, T.L. Gilchrist, Longman Scientific Teehinai.
- 11. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
- 12. Contemporary Heterocyclic Chemistry, Q.R. Newkome and W.W. Paudler, Wiley Inter Science.
- 13. An introduction to the Heterocyclic compounds, Linds, R.M. Acheson, John Wiley.
- 14. Comprehensive Heterocyclic Chemistry, A.R. Kalriliky and C.W. Rees, eds. Pergamon press.
- 15. Natural produds; Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthirope and J.B. Harbome, Longman, Essex.
- 16. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
- 17. Steroselective synthesis; a Practical Approach, Nogradi, VCH.
- 18. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 19. Chemistry Biological and Pharmacological Properties of Medicinal plants from the Americas. Ed. Kurt Hosieumann, M.P. Gupta and A. Marston. Harwood Academic Publishers.
- 20. Introduction lo Flavonoids, B.A. Bohm, Harwood Academic Publishers.
- 21. New trends in natural product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers.
- 22. Insecticides of Natural Origin, SukhDev, Harwood Academic Publishers.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

- A Internal written Examination 20 Marks (1 Hr)
- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

# Chemistry M.Sc. Semester – IV EC 4 (Physical ChemistrySpecial)

#### Full Marks - 70

Time :03 Hours

- 1. Eight questions are to be set atleast one question from each chapter.
- 2. Question 1 will be objective type question (MCQ)/True-False/Fill in the blanks etc. 10 question of 1 mark each (Compulsory)
- 3. Any Four questions out of the remaining Seven questions to be answered 15 marks each.

#### I. Potential Energy Surfaces

Mechanism of activation, Potential Energy Surface for three atom reaction. Potential Energy curve for successive reaction, proportions of Potential Energy Surfaces. Inter conversion of translational and vibrational energies, combination of atoms, orthopara conversion. Activated state of three atom and four atom reaction, Potential Energy refile, reaction co-ordinate. Transmission co-efficient.

### **II. Kinetics of Condensed Phase Reactions**

Rate determining steps in diffusion controlled reactions and activation controlled reactions, Stokes Einstein equation and dependence of rate constant on co-efficient of viscosity of medium, Kinetics of ionic reactions in solution-electrostatic contribution to free energy in single and double spherical models of activated complex, entropy of activation for ion-ion reaction; Kinetics of dipole-dipole reaction, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, BronstedBjerrum equation.

#### **III. Catalysis and Oscillation**

Kinetics of catalytic reactions, theory of acid-base catalysis, Van't Hoff and Arrhensius complexes.Protogenic and Protophilic mechanisms.Effect of salt on acid-base catalysis, autocatalysis, non-competitive and competitive inhibitors, Bronsted catalysis law, rate of reaction and acidity function.Liner free energy relationship, Hammet equation.Meaning of subsitiuent constant and reaction constant in organic reactions.Reactions in Biological system.Oscillating reaction, Lotka-Voltera model.B-Z reaction.

#### **IV. Study of Fast Reaction**

Photo Physical Chemistry – Flash Photolysis.Relaxation technique, Nuclear Magnetic Resonance Method. Molecular beam and Shock – tube Kinetics, flow method. Reactions of Protons, Electrons metal ions.

#### V. Electrodes Kinetics

Faradaic and non-faradaic current, Rate law in faradaic process, Current density, Factors affecting electrode reaction Types of over voltage, Polarisation, Polarisation curves, Electric Potential. Derivation of Nernst equation (i) On thermodynamic consideration and (ii) by Kinetic approach Tafel plot. Bukte-Volmor equation, Nernst diffusion layer treatment, exchange current density, Stoichiometric number, Conce of rate determining steps. Energy Barriers for multi steps reactions.

#### VI. Electrode Deposition and Corrosion Processes

Eletrocatalysis – electrocalaytic rate, Eletrocatalysis in redox system. Total deposition current density, Time variation of the over potential and rate determining step in electrode deposition total over potential for electrode deposition at steady state. Hydrogen over voltage, rate determining stop of the hydrogen evolution reaction, determination of reaction order with respect to H+ ion in solution.Corrosion current.Elctro nation current and Corrosion potential, electro nation reaction, corrosion and stability of metals.

### Sessional Internal Assessment (SIA) Full Marks - 30 Marks

A – Internal written Examination – 20 Marks (1 Hr)

- B Written Assignment 05 Marks
- C Over All Performance including Regularity 05 Marks

M.Sc.

### Semester - IV

## EC 5 (Practical)

# (Inorganic Chemistry Special)

Full Marks - 100

**Time :06 Hours** 

Two questions are to be set

- I. Preparation of inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods.
  - (a) Preparation and characterization of Cr (III) complexes
  - (i)  $[Cr(H_2O)_6]NO.H_2O$
  - (ii)  $[Cr(H_2O)_4Cl_2]Cl.H_2O$
  - (iii) Cr(acac)<sub>3</sub>
  - (b) (i) Purification of inorganic complexes using techniques such as crystallization, Volatilisation etc.
     (ii) Tests for purity M.P. TLC, Metal analysis etc.
  - (c) Preparation and study of cis and trans isomers of bis (glycinato) copper (II)
    - (a) Cis (glycinato) Cu (II) monohydrate
    - (b) Trans-(glycinato) Cu (II) monohydrate (IR Spectroscopy)
    - (c) Preparation of mercury tetrathiocyanatocobaltate : Hg [Co(CNS)<sub>4</sub>]

### II. Flame photometric determination

- (a) Sodium and Potassium when present together
- (b) Li / Ca / Ba / Sr

### **III. Naphelometric determinations**

- (a) Sulphate
- (b) Phosphate
- (c) Silver

### IV. Determination of

- (a) Manganese / Chromium / Vanadium in steel sample by spectrophotometric method.
- (b) Ni / Mo/ W/ V/ U by extractive spectrophotometric method.

Experiments - 80 Marks

Viva-Voice – 10 Marks

Notebook – 10 Marks

M.Sc.

### Semester – IV

# EC 5 (Practical)

# (Organic Chemistry Special)

### Full Marks - 100

Time :06 Hours

Two questions are to be set

### I. Quantitative Analysis

### Some illustrative exercises are given below :

- 1. Estimation of phenol / aniline using bromate bromide solution / or acetylation method.
- 2. Estimation of carbonyl group by using 2, 4-dinitrophenyl hydrazine.
- 3. To estimate nitrogen in the given sample by Kjeldahl method.
- 4. To estimate sulphur in the given sample by the Na<sub>2</sub>CO<sub>3</sub>-KNO<sub>3</sub> fusion method.
- 5. To estimate sulphur in the given sample by Messenger's method.
- 6. To estimate halogen in the given sample by the alkaline reduction method (modified stepanow method).
- 7. To determine the percentage or number of hydroxyl group in the given sample by the acetylation method.
- 8. To determine the percentage or number of phenolic groups in the given sample by the acetylation method.
- 9. To determine the percentage or number of phenolic groups in the given sample by the Zeisel's method.
- 10. To determine the iodine number of the given fat or oil sample.

Experiments - 80 Marks

Viva-Voice - 10 Marks

Notebook - 10 Marks

M.Sc.

### Semester - III

### EC 5 (Practical)

# (Physical Chemistry Special)

### Full Marks - 100

Time :06 Hours

Two questions are to be set

### I. Chemical Kinetics

- (a) To study the kinetics of alkaline hydrolysis of an ester in aqua-organic solvent system with respect to effect the solvent composition and dielectric constant on rate constant.
- (b) To determine the rate constant of the reaction between  $K_2S_2O_8$  and KI at two different temperature and hence to determine the energy of activation of the reaction.

### II. Thermochemistry

- (a) Determination of basicity of polybasic acid.
- (b) Determination of heat of displacement of Cu by Zn and  $Cu^{+2}$  salt solution.
- (c) Determination of heat of hydration of  $Na_2SO_4$  to  $Na_2SO_4$ .10H<sub>2</sub>O.

### **III. Distribution Law**

Determination of equilibrium constant for the reaction  $KI + I_2 = KI_3$ .

### IV. Thermodynamics and Surface Chemistry

- (a) To study the adsorption of acetic acid on charcoal.
- (b) To determine the partial molar volume of solutions of simple salts and to study its variation with concentration.

### V. Viscosity and Surface Tension

- (a) To determine the radius of a molecule from viscosity measurement.
- (b) To determine the parachor of –CH<sub>2</sub>, C and H.

Experiments - 80 Marks

Viva-Voice - 10 Marks

Notebook - 10 Marks

# M.Sc.

### Semester - IV

# **Project Work (End Sem.)**

### Full Marks – 100 (Written component = 80 Marks + Viva-voce = 20 Marks)

### The paper will consist of

- (a) Field work / Lab work related to the project.
- (b) Preparation of dissertation based on the work undertaken.
- (c) Presentation of project work in the seminar on the assigned topic in the Department of Chemistry, Kolhan University, Chaibasa& opened viva there on.
- NB : The students will select topics for the project work in consultation with a teacher of the Department.

### **TOPICS**

Project work related to the following Industrial / Socially relevant topics may be given to the students.

- (a) Environmental study such as (i) Analysis of Water, Soil, Air etc.
- (b) Industrial goods analysis such as
  - (i) Analysis of Cement.
  - (ii) Analysis of Haematite.
  - (iii) Analysis of minerals available in Jharkhand State.
  - (iv) Synthesis of useful commercial products based on raw materials available in Jharkhand State such as Lac, Limestone etc.
  - (v) Isolation of constituents of medicinal plants available Jharkhand State.

Each student has to submit three copies of the dissertation work duly forwarded by HOD of Department / Principal of the college. The forwarded copies will be submitted to the Department of Chemistry, Kolhan University, Chaibasa. (Seven days before the seminar)

### NB : the seminar will be held in the Department of Chemistry, Kolhan University, Chaibasa.

**Time :06 Hours**