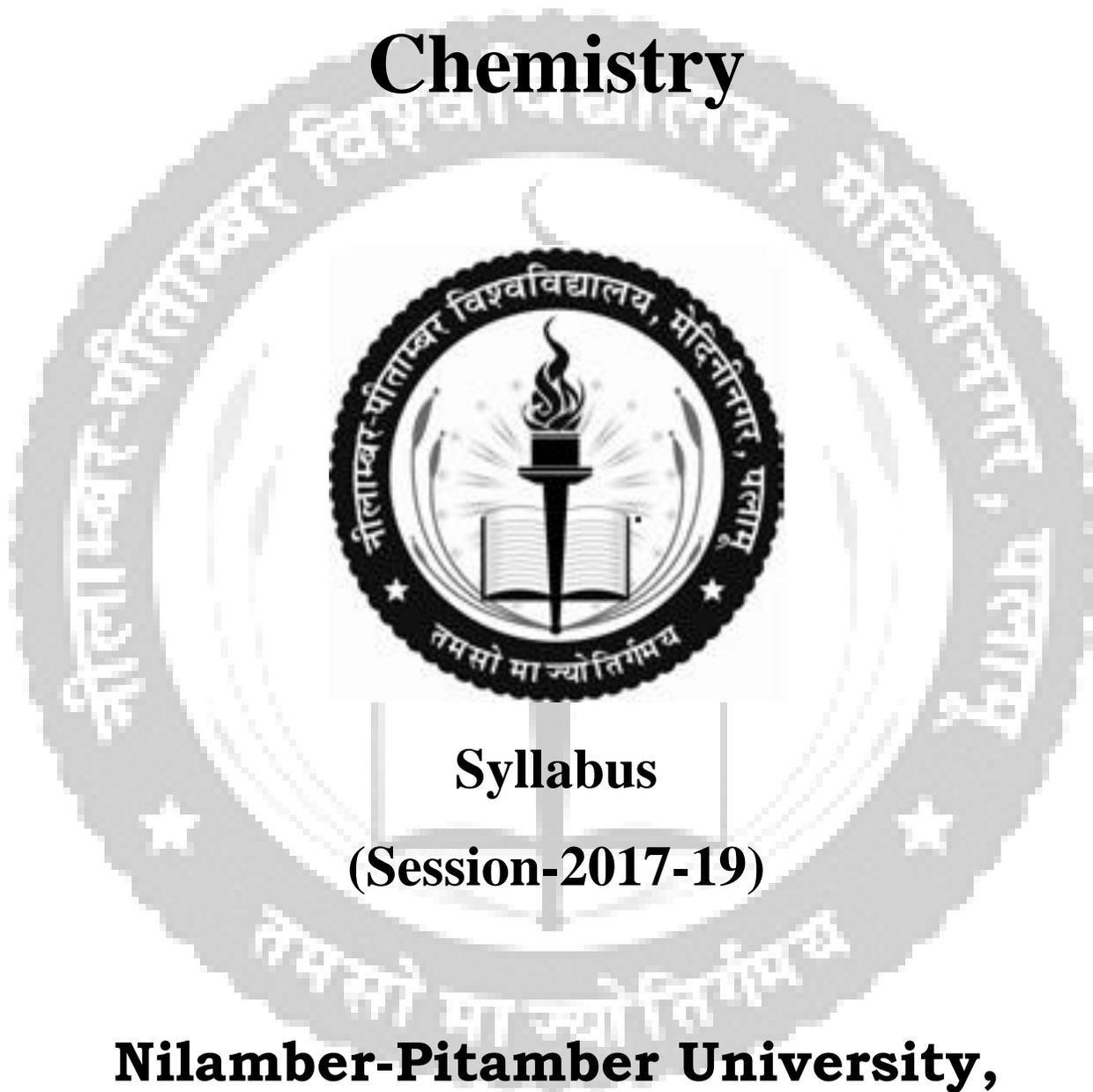


# **CBCS Four Semester Course of PG Programme for Chemistry**



**Syllabus**

**(Session-2017-19)**

**Nilamber-Pitamber University,  
Medininagar**

**Palamu, Jharkhand-822 101**



## Semesterwise Distribution of Course

### Course Structure for M.Sc. Programme

Semester	Course	Credit	Hrs./Week
I	FC (Compulsory) – (FC-I)	5	5 (L) + 1 (T)
	Core Course – 1 (CC-1)	5	5 (L) + 1 (T)
	Core Course – 2 (CC-2)	5	5 (L) + 1 (T)
	Core Course (P) – 3 [CC (P)-3]	5	10
II	Elective Course (SE) (EC-1)	5	5 (L) + 1 (T)
	CC-4	5	5 (L) + 1 (T)
	CC-5	5	5 (L) + 1 (T)
	CC(P)-6	5	10
III	CC-7	5	5 (L) + 1 (T)
	CC-8	5	5 (L) + 1 (T)
	Elective (GE/DC) (EC-2)	5	5 (L) + 1 (T)
	EC(P)-3	5	10
IV	CC-9	5	5 (L) + 1 (T)
	Elective (GE/DC) (EC-4)	5	5 (L) + 1 (T)
	EC(P) – 5	5	5 (L) + 1 (T)
	Project	5	10

**Chemistry**  
**M.Sc. Semester-1**  
**FC – Compulsory (FC-1)**

Full Marks: 70+30

Time : 03 Hours

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Stereochemistry and Bonding in Main Group Compounds 09 Hrs**  
VSEPR, Walsh diagrams (tri-atomic molecules of type  $AH_2$ ), dp-pp bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules, Atomic Inversion, Berry Pseudorotation.
- II Nature of Bonding in Organic Molecules 12 Hrs**  
Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes, tautomerism.  
Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of  $\pi$ -molecular orbitals, annulenes, antiaromaticity,  $\Psi$ -aromaticity, homo-aromaticity, PMO approach.  
Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.
- III Stereochemistry 16 Hrs**  
Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, 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.  
Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

**IV Introduction to Exact Quantum Mechanical Results 09 Hrs**

The Schrodinger equation 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.

**V Unifying Principles 12 Hrs**

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

**VI Metal-Ligand Equilibria in Solution 12 Hrs**

Step wise 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.

**Books Suggested**

1. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
2. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
3. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
4. Quantum Chemistry, Ira N. Levine, Prentice Hall.
5. Chemical Applications of Group Theory, F. A. Cotton.
6. Physical Methods in Chemistry, R.S. Drago, Saunders College.
7. Introduction to Molecular Spectroscopy, Q.M. Barrow, McCraw Hill.

**Chemistry**  
**M.Sc. Semester-1**  
**Core Course – 1 (CC-1)**

Full Marks: 70+30  
Time : 03 Hours

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Reaction Mechanism of Transition Metal Complexes 25 Hrs**  
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, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions
- II Metal  $\pi$ -Complexes 16 Hrs**  
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 phosphine as ligand.
- III Metal-Ligand Bonding 08 Hrs**  
Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.
- IV Electronic Spectra and Magnetic Properties of Transition Metal Complexes 15 Hrs**  
Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states), calculations of  $Dq$ ,  $B$  and  $b$  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.
- V Metal Clusters 06 Hrs**  
Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

**Books Suggested**

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row;
3. Chemisiry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
4. Inorganic Electron ioSpeci roscopy, A. B. P. Leve r, Elsevier.
5. Magnetochemistry, R.L. Cariin, Springer Vertag,
6. Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

**Chemistry**  
**M.Sc. Semester-I**  
**Core Course – 2 (CC-2)**

Full Marks: 70+30  
Time : 03 Hours

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

**I Reaction Mechanism: Structure and Reactivity** **20 Hrs**

Types of mechanisms, types of reactions, 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, isotope effects. Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

**II Aliphatic Nucleophilic Substitution** **20 Hrs**

The  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$  and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by R and a bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

The  $S_Ni$  mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

**III Aliphatic Electrophilic Substitution** **07 Hrs**

Bimolecular mechanisms-  $S_E2$  and  $S_Ei$ . The  $S_{O2}$  mechanism, electrophilic substitution accompanied by double bond shifts.

Effect of substrates, leaving group and the solvent polarity on the reactivity.

**IV Aromatic Electrophilic Substitution** **08 Hrs**

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.

**V Aromatic Nucleophilic Substitution****03 Hrs**

The  $S_NAr$ ,  $S_{NO}$ , benzyne and  $S_{RO}$  mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

**VI Free Radical Reactions****12 Hrs**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**Books Suggested**

1. Advanced Organic Chemistry-Reactions, 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 Reactions, H. O. House, Benjamin.
7. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji 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.

**Chemistry**  
**M.Sc. Semester-1**  
**Core Course (P) – 3 [CC(P)-3]**

**Full Marks: 100**

**Time : 06 Hrs**

1. Cent per cent quantitative Analysis of Cement
2. 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) Managnese in steel by sodium bismuthate method.
3. **Organic Qualitative**  
Identification of organic compounds containing one functional group using Chemical Analysis
4. **Preparation of organic compounds using methods not involving more than two steps.**  
**Some of the experiments listed below:**
  - (i) Preparation of methyl Orange
  - (iv) Preparation of Martius yellow
  - (vi) Preparation of p-nitro aniline from acetanilide
  - (viii) Preparation of Cinnamic acid from Benzaldehyde
5. **Estimation of Glucose**

**Chemistry**  
**M.Sc. Semester-II**  
**Elective Course (SE) (EC-1)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

**I Introduction to Computers and Computing 10 Hrs**

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

**II Computer Programming in C Language 20 Hrs**

Elements of the Computer Language Constants and variables and data types. Operators and Expressions, Arithmetical, Relational, Logical, Assignment, Increment and Decrement operators. Input and output statements. Branching statements such as (if-else, goto, switch) statements. Decision making and looping (while, for, do). Arrays (one dimensional and two dimensional arrays). Sorting of data in an array. Function (user defined functions).

**III Programming in Chemistry 25 Hrs**

Development of small computer codes involving simple formulae in chemistry, such as vander Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations 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 15 Hrs**

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Packages- MS-Word, MS-Excel, ORIGIN, MATLAB.

**Books Suggested**

- 1 Comdex Computer Course kit (XP Edition), Vikas 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, Pragati Prakshan

**OR**  
**BIO-CHEMISTRY**  
**GROUP-A**

- I Metal Ions in Biological Systems** **03 Hrs**  
Essential and trace metals. Na<sup>+</sup>/K<sup>+</sup> Pump  
Role of metals ions in biological processes,
- II Bioenergetics and ATP Cycle** **08 Hrs**  
DNA polymerisation, glucose storage, metal complexes In transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems.
- III Transport and Storage of Dioxygen** **05 Hrs**  
Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.
- IV Electron Transfer in Biology** **08 Hrs**  
Structure and function of metalloproteins in electron transport processes - cytochromes and iron-sulphur proteins, synthetic models
- Nitrogenase** **05 Hrs**  
Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

**GROUP B**

- I Enzymes and Mechanism of Enzyme Action** **02 Hrs**  
Basic considerations. Proximity effects and molecular adaptation.
- Enzymes** **10 Hrs**  
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 Koshland'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 Lineweaver-Burk plots, reversible and irreversible Inhibition.
- Mechanism of Enzyme Action** **06 Hrs**  
Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.
- II Kinds of Reactions Catalysed by Enzymes** **08 Hrs**  
Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Addition and elimination reactions, enolic intermediates in isomerization reactions, p-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.
- III Co-Enzyme Chemistry** **05 Hrs**  
Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal

phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipolic acid, vitamin B<sub>12</sub>. Mechanisms of reactions catalyzed by the above cofactors.

#### **IV Biotechnological Applications of Enzymes** **10 Hrs**

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 food 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.

#### **Books Suggested**

1. Principles of Bioinorganic Chemistry, S.J. Lippard and 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 vols I and II. ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 3S ed. J.J. Lippard, Wiley.
5. Bioorganic 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 Applications, Ed. Collin J Suckling, Chapman and Hall.
8. Enzyme Mechanisms Ed, M. 1. Page and A. Williams, 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. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.

**OR**

#### **PHOTO IN-ORGANIC CHEMISTRY**

#### **I Excited States of Metal Complexes** **15 Hrs**

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

#### **II Ligand Field Photochemistry** **15 Hrs**

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zerozero spectroscopic energy, development of the equations for redox potentials of the excited states.

#### **III Redox Reactions by Excited Metal Complexes** **25 Hrs**

Energy transfer under conditions of weak interaction and strong interaction-exciplep formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-

phenanthroline complexes), illustration of reducing and oxidising character of Ruthenium<sup>2+</sup>(bipyridal complex, comparison with Fe(bipy)<sub>3</sub>; role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light

**VI Metal Complex Sensitizers 15 Hrs**

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

**Books Suggested**

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J. Chem. Educ., vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
4. Coordination Chem. Revs., 1981, vol. 39, 121, 131; 1975, 15, 321; 1990, 97, 313.
5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements of Inorganic Photochemistry, G. J. Ferraudi, Wiley.

**OR**

**ORGANIC**

**I Acids, Bases, Electrophiles, Nucleophiles and Catalysis 15 Hrs**

Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The ex-effect. Ambivalent nucleophiles. Acid-base catalysis- specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non- covalent binding-micellar catalysis.

**II Steric and Conformational Properties 10 Hrs**

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

**III Nucleophilic and Electrophilic Reactivity 10 Hrs**

Structural and electronic effects on S<sub>N</sub>1 and S<sub>N</sub>2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance: Electron transfer nature of S<sub>N</sub>2 reaction. Nucleophilicity and S<sub>N</sub>2 reactivity based on curve- crossing model. Relationship between polar and electron transfer reactions. S<sub>RO</sub> mechanism. Electrophilic reactivity, general mechanism. Kinetic of S<sub>E</sub>2-Ar reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

**IV Radical and Pericyclic Reactivity 10 Hrs**

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

## V Supramolecular Chemistry

25 Hrs

Properties of covalent bonds - bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond. Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixerenes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

### Books Suggested

1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. 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 to Theoretical Organic Chemistry and Molecular Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, Concepts and Perspectives, J. M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

**Chemistry**  
**M.Sc. Semester-II**  
**Core Course – 4 (CC-4)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

**I. Quantum Chemistry** **30 Hrs**

A Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

B Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

C Electronic Structure of Atoms

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

D Molecular Orbital Theory

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

**II. Classical Thermodynamics** **15 Hrs**

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic

strength. Gibb's Duhem equation, Nernst heat theorem and its applications, Determination of absolute entropy Maxwell's thermodynamic relation.

### III Chemical Dynamics

25 Hrs

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

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov -Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann - Hinshelwood and Rice-Ramsperger - Kassel-Marcus [RRKM] theories of unimolecular reactions).

#### 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 Valence, R. McWeeny, ELBS.
5. Chemical Kinetics, K. J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum
8. Modern Electrochemistry Vol. I and 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.

**Chemistry**  
**M.Sc. Semester-II**  
**Core Course – 5 (CC-5)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

**I Symmetry and Group Theory In Chemistry 25 Hrs**

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

**III Microwave Spectroscopy 05 Hrs**

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

**IV Vibrational Spectroscopy 20 Hrs**

**A. Infrared Spectroscopy**

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; 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).

**V Electronic Spectroscopy 10 Hrs**

**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 transitions, 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, spectra of transition metal complexes, charge-transfer spectra.

## VI X-ray Diffraction

10 Hrs

Bragg condition, -Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

### Books Suggested

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

**Chemistry**  
**M.Sc. Semester-II**  
**Core Course (P) – 6 [CC(P)-6]**

**Full Marks: 100**

**Time : 06 Hrs**

**1. Measurement of density of gases and vapours**

- (a) Victor Meyer's Method Determination of Molecular weight of Acetone, Chloroform, Benzene, (Mixture).
- (b) Duma's Method Determination of molecular weight of acetone, Carbon-Tetrachloride.

**2. Determination of Molecular weight of substances**

- (a) Beckmann's freezing point Method
- (b) Beckmann's Boiling point method.

**3. Viscosity of liquids and solution by ostwald tube**

Determination of percentage composition of a mixture of two liquids.

**4. Surface Tension of liquids and solutions**

- (a) Study of the effect of conc. on surface tension of acetic acid and Sod. chloride solutions.
- (b) Determination of Parachor.

**5. Thermochemistry**

- (a) Determination of water equivalent of a calorimeter
- (b) Determination of the Heat of Neutralization of :
  - (i) Strong acid and strong base (HCl and NaOH)
  - (ii) Weak acid and strong base (NaOH and  $\text{CH}_3\text{COOH}$ ).
- (c) Determination of Heat of solution of Potassium Nitrate
- (d) Determination of basicity of succinic Acid by Thermochemical Method.

**6. Order of Reaction**

- (a) Determination of the rate constant of hydrolysis of an ester with an acid (Methyl acetate and HCl).
- (b) Determination of the rate constant of saponification of ethyl acetate by NaOH.

**7. Partition Co-efficient**

- (a) Determination of partition coefficient of:
  - (i) Benzoic acid between water and Benzene
  - (ii) Iodine between water and carbon tetrachloride

**9. 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 acid and strong base ( $\text{CH}_3\text{COOH}$  and NaOH)

**Chemistry**  
**M.Sc. Semester-III**  
**Core Course – 7 (CC-7)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Ultraviolet and Visible Spectroscopy 10 Hrs**  
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 heterocyclic compounds.
- II Infrared Spectroscopy 10 Hrs**  
Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids and polymeric materials.
- III Nuclear Magnetic Resonance Spectroscopy 14 Hrs**  
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, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique.
- Carbon-13 NMR Spectroscopy 08 Hrs**  
General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.
- IV Mass Spectrometry 10 Hrs**  
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 spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.
- V Electron Spin Resonance Spectroscopy 09 Hrs**  
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  $\text{PH}_4$ ,  $\text{F}_2^-$  and  $[\text{BH}_3]^-$ .

## VI Mössbauer Spectroscopy

09 Hrs

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

### Books 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. Craddock, ELBS
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry of R.L. Carlin vol. 5, Dekker
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
8. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpuech and Q.J. Martin, Heyden.
9. Spectrometric identification of Organic Compounds, R. M. Silverstein, Q. C. Bassler and T. C. Morrill, John Wiley
10. Introduction to NMR Spectroscopy. R. J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
12. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill.

**Chemistry**  
**M.Sc. Semester-III**  
**Core Course – 8 (CC-8)**

**Full Marks: 70+30**

**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

**I Environment**

**10 Hrs**

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. Biodistribution of elements.

**II Hydrosphere**

**20 Hrs**

Chemical composition 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, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOO, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chloine demand. Purification and treatment of water.

**III Soils**

**05 Hrs**

Composition, micro and macro nutrients, Pollution'- fertilizers, pesticides, plastics and metals. Waste treatment.

**IV Atmosphere**

**15 Hrs**

Chemical composition of atmosphere - particles, ions and radicals 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, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

**V Industrial Pollution****10 Hrs**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

**VI Environmental Toxicology****10 Hrs**

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three mile island, Sewozo and Minamata disasters.

**Books Suggested**

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
3. Environmental Chemistry, A. K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Standard Method of Chemical Analysis, FJ. Weleher Vol. III. Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Crealchman, Gordon and Breach Science Publication.
8. Environmental Chemistry, C. Baird, W. H. Freeman.

**Chemistry**  
**M.Sc. Semester-III**  
**In-Organic**  
**Elective (GE/DC) (EC-2)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- |   |               |
|---|---------------|
| <b>I Alkyls and Aryls of Transition Metals</b>  | <b>05 Hrs</b> |
| Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis   |               |
| <b>II Compounds of Transition Metal-Carbon Multiple Bonds</b>   | <b>15 Hrs</b> |
| Alkylidenes, alkylidyne, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis  |               |
| <b>III Transition Metal <math>\pi</math>-Complexes</b>  | <b>18 Hrs</b> |
| Transition metal $\pi$ -complexes with unsaturated organic molecules, alkenes, alkynes, atlyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis |               |
| <b>IV Transition Metal Compounds with Bonds to Hydrogen</b>   | <b>07 Hrs</b> |
| Transition Metal Compounds with Bonds to Hydrogen.  |               |
| <b>I Metals in Medicine</b>   | <b>05 Hrs</b> |
| Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs   |               |
| <b>III Homogeneous Catalysis</b>  | <b>14 Hrs</b> |
| Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.   |               |
| <b>IV Fluxional Organometallic Compounds</b>  | <b>06 Hrs</b> |
| Fluxionality and dynamic equilibria in compounds such as $h^2$ -olefin, $h^3$ allyl and dienyl complexes  |               |

**Books Suggested**

- 1 Principles and Application of Organotransition 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.

**Chemistry**  
**M.Sc. Semester-III**  
**Organic**  
**Elective (GE/DC) (EC-2)**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Terpenoids and Carotenoids** **15 Hrs**  
Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral,  $\alpha$ -Terpeneol, Zingiberene, Santonin, Bisabolene acid and (3-Carotene).
- II Alkaloids** **14 Hrs**  
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, Reserpine
- III Six-Membered Heterocycles with one Heteroatom** **06 Hrs**  
Synthesis and reactions of pyrytium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones
- IV Heterocyclic Systems Containing S & As** **12 Hrs**  
Heterocyclic rings containing phosphorus: introduction, nomenclature, Synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing As introduction, synthesis and characteristics of 5- and 6 membered ring systems.
- II Principles of Reactivity** **07 Hrs**  
Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.
- III Kinetic Isotope Effect** **06 Hrs**  
Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

#### IV Structural Effects on Reactivity

10 Hrs

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of  $\rho$ -values. Reaction constant  $\rho$ . Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model,  $\sigma$ ,  $\sigma^+$  and  $\sigma^-$ -scales.

#### Books Suggested

1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. 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 to Theoretical Organic Chemistry and Molecular Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, Concepts and Perspectives, J. M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.



**Chemistry**  
**M.Sc. Semester-III**  
**Physical**  
**Elective (GE/DC) (EC-2)**

**Full Marks: 70+30**

**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Diffraction of X-rays by crystals 08 Hrs**  
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 15 Hrs**  
Free electron theory, band theory, Fermi level, Brillouin zone, wave function for electrons in solids, metallic conductors, insulator, semi conductors (intrinsic & extrinsic), properties of junctions.
- III Polymer 09 Hrs**  
Polymer solution, thermodynamics of polymer solutions, molar mass and molar mass distribution, methods of measuring molar masses, micelle formation and hydrophobic interaction.
- IV Electrically conducting polymers 08 Hrs**  
Electrically conducting polymers electrochemical polymerization, band structure of polymers, mechanism of conduction in polymers, doping of polymers, application of conduction polymers.
- V Potential Energy Surfaces 15 Hrs**  
Mechanism of activation, potential energy surface for three atom reaction, Potential energy curve for successive reactions, Properties of potential energy surfaces, Inter conversion of translational and vibrational energies, Combination of atoms, Orthopara conversion, Activated state of three atom and four atom reactions, Potential energy profile, reaction coordinate, Transmission coefficient, non-adiabatic reaction.
- VI Study of Fast Reactions 15 Hrs**  
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.

**Chemistry**  
**M.Sc. Semester-III**  
**In-Organic**  
**EC(P)-3**

**Full Marks: 100**  
**Time : 06 Hrs**

**Credit : 5**

1. Qualitative separation and determination of the following pairs of metal ion using gravimetric and volumetric methods
  - a)  $\text{Ag}^+(\text{g})$  and  $\text{Cu}^{2+}(\text{v})$
  - b)  $\text{Cu}^{2+}(\text{g})$  and  $\text{Zn}^{2+}(\text{v})$
  - c)  $\text{Fe}^{3+}(\text{g})$  and  $\text{Ca}^{2+}(\text{v})$
  - d)  $\text{Mg}^{2+}(\text{g})$  and  $\text{Ca}^{2+}(\text{v})$
2. Semi micro qualitative analysis of a mixture containing five cations of rare element and insolubles.
  - a) Rare element Tl, W Sc Mo, Ti, Zr Ce, Tb V, V, Lx
  - b) Insoluble  $\text{PbSO}_4$ ,  $\text{SrSO}_4$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{Cr}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{SnO}_2$ ,  $\text{ThO}_2$ ,  $\text{WO}_3$

**Chemistry**  
**M.Sc. Semester-III**  
**Organic**  
**EC(P)-3**

**Full Marks: 100**  
**Time : 06 Hrs**

**Credit : 5**

**Group A**

Characterization of organic compounds, The students expected to carry out analysis of the components of binary org. mixture (liquid-liquid, liquid-solid & solid-solid) the students should also check the purity of the separated components on TLC plates.

**Group-B**

1. To determine the percentage or number of phenolic groups in the given sample by the acetylation method.
2. To determine the percentage or number of methoxyl groups in the given sample by the Zeisel's method.
3. To determine the iodine number of the given fat or oil sample.



**Chemistry**  
**M.Sc. Semester-III**  
**Physical**  
**EC(P)-3**

**Full Marks: 100**  
**Time : 06 Hrs**

**Credit : 5**

**I Conductometry**

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

**II. Potentiometry**

1. To determine the solubility and solubility product of AgCl in water
2. To determine the E<sup>0</sup> of Zn/Zn<sup>++</sup>, Cu/Cu<sup>++</sup> ELECTRODES.
3. To determine the basicity of a polybasic acid and its dissociation constant.
4. To investigate the complex formed between CuSO<sub>4</sub> and NH<sub>3</sub>.

**III. Polarimetry**

1. To analyse a mixture of glucose and sucrose
2. To study the inversion of cane sugar in acid medium.

**IV. Refractometry**

1. To verify mixture law of refraction
2. To determine the composition of an unknown solution.

**V. Cryoscopy**

1. To determine the activity of a non-electrolyte by freezing point method
2. To determine the mean activity co-efficient of KCl by freezing point method.

**Chemistry**  
**M.Sc. Semester-IV**  
**CC-9**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Introduction 15 Hrs**  
Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations - dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.
- II Errors and Evaluation 15 Hrs**  
Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.
- III Food Analysis 12 Hrs**  
Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.
- IV Analysis of Water Pollution 16 Hrs**  
Origin of waste water, types, water pollutants and their effects. Sources of water pollution-domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.
- V Analysis of Soil, Fuel, Body Fluids and Drugs 12 Hrs**  
(a) Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

- (b) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating valuesgrading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.
- (c) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis- (d) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

### **Books Suggested**

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W. B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W. B. Saunders.
6. Principles of Instrumental Analysis, D.A. Skoog, W. B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
11. Analytical Chemistry, G.D. Christian, J. Wiley.

**Chemistry**  
**M.Sc. Semester-IV**  
**In-Organic**  
**Elective (GE/DC) [EC-4]**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- |            |   |               |
|------------|---|---------------|
| <b>I</b>   | <b>Metal Storage Transport and Biomineralization</b>  | <b>07 Hrs</b> |
|            | Ferritin, transferrin, and siderophores   |               |
| <b>II</b>  | <b>Calcium in Biology</b>   | <b>10 Hrs</b> |
|            | Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins  |               |
| <b>III</b> | <b>Metalloenzymes</b>   | <b>20 Hrs</b> |
|            | Zinc enzymes - carboxypeptidase and carbonic anhydrase. Iron enzymes - catalase, peroxidase and cytochrome P-450. Copper enzymes - superoxide dismutase. Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin B12 |               |
| <b>IV</b>  | <b>Metal-Nucleic Acid Interactions</b>  | <b>08Hrs</b>  |
|            | Metal ions and metal complex interactions. Metal complexes - nucleic acids  |               |
| <b>II</b>  | <b>Supramolecular Chemistry</b>   | <b>25 Hrs</b> |
|            | Concepts and language.  |               |
|            | (A) Molecular recognition : Molecular receptors for different types of molecules 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, supramolecular electronic, ionic and switching devices.  |               |
|            | Some example of self-assembly in supramolecular chemistry   |               |

**Books Suggested**

- 1 Principles of Bioinorganic Chemistry, S.J. Lippard and 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 vols 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.

**Chemistry**  
**M.Sc. Semester-IV**  
**Organic**  
**Elective (GE/DC) [EC-4]**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**  
**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Steroids 20 Hrs**  
Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry.  
Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Biosynthesis of steroids.
- II Six-Membered Heterocycles with Two or More Heteroatoms 05Hrs**  
Synthesis and reactions of diazines, triazines, tetrazines and thiazines
- III Seven- and Large-Membered Heterocycles 05 Hrs**  
Synthesis and reactions of azepines, diazepines.
- IV Structure Determination and Synthesis of Vit. A, B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub>, Vit. C and Vit. D. 20 Hrs**
- V Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory 20 Hrs**  
Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and *ab initio* and density functional methods. Scope and limitations of several computational programmes.  
Quantitative MO theory - Huckel molecular orbital (HMO) method as applied to ethene, 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 ethene, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.  
Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curvecrossing model-nature of activation barrier in chemical reactions

## Books Suggested

1. Heterocyclic Chemistry Vol. 1-3, R. R. Supta, M. Kumar and V Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, Q. R. Newkome and W. W. Paudler, Wiley-Interscience.
6. An introduction to the Heterocyclic Compounds. Linds, R. M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, eds. Pergamon Press.
8. Natural Products; Chemistry and Biological Significance, J. Mann, R. S. Davidson, J.B. Hobbs, D.V. Banthiropo and J. B. Harborne, Longman, Essex.
9. Organic Chemistry, Vol 2, I.L. Finar, ELBS.
10. Stereoselective Synthesis; A Practical Approach, M. Nogradi, VCH.
11. Rodd's Chemistry of Carbon Compounds. Ed. S. Coffey, Elsevier.
12. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hosieitmann, M. P. Gupta and A. Marston, Harwood Academic Publishers.
13. Introduction to Flavonoids. B.A. Bohm, Harwood Academic Publishers.
14. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M I Choudhary, Harwood Academic Publishers.

**Chemistry**  
**M.Sc. Semester-IV**  
**Physical**  
**Elective (GE/DC) [EC-4]**

**Full Marks: 70+30**  
**Time : 03 Hours**

**Total Lecturer : 70 Hours**

**Credit : 5**

**Eight questions are to be set out of which five are to be answered.**

- I Super conductivity 11 Hrs**
- Super conductivity meissner effect, microscopic theory of superconductivity, conventional organic and high temp, superconductors, fullerenes, applications of superconductors.
- Transformation in crystals - thermodynamics of transformation, order-disorder transitions, martensitic transition, polymorphic transformation
- II Specific heat of solids 11 Hrs**
- Specific heat of solids classical theory, quantum theory of specific heats-Einstein and Debye theories, characteristic temp and its calculation, T-law. Solid state reactions, laws governing nucleation, homogeneous and heterogenous nucleation, thermodynamic barrier.
- III Polymer liquid crystal 11 Hrs**
- Polymer liquid crystal nematic, cholesteric and smectic phases, liquid crystalline order of the main chain and of the side groups in polymers, synthesis and properties of polymer liquid crystals, liquid crystalline order in biological materials.
- IV Surface chemistry 12 Hrs**
- Surface chemistry surface films, BET isotherm for, multilayers & its derivation, kinetics of surface processes, unimolecular and bimolecular surface reactions, electrocapillarity, electrokinetic effects, statistical mechanics of adsorption.

## VI Kinetics of Condensed Phase Reactions

25 Hrs

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 reactions; Kinetics of dipole-dipole reaction, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted-Bjerrum equation.

### Books suggested

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

**Chemistry**  
**M.Sc. Semester-IV**  
**In-Organic**  
**EC(P)-5**

**Full Marks: 100**  
**Time : 06 Hrs**

**Credit : 5**

**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 six to eight simple inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods**

- (a) Preparation of Cobalt (III) complexes
  - (i)  $[\text{Co}(\text{NH}_3)_5 \text{Cl}] \text{Cl}_2$
  - (ii)  $[\text{Co}(\text{NH}_3)_5 \text{NO}_2] \text{Cl}_2$
  - (iii)  $[\text{Co}(\text{NH}_3)_5 \text{ONC}] \text{Cl}_2$
- (b) Preparation and characterisation of Cr(III) complexes
  - (i)  $[\text{Cr}(\text{H}_2\text{O})_6] \text{NO}_3 \text{H}_2\text{O}$
  - (ii)  $[\text{Cr}(\text{H}_2\text{O})_4 \text{Cl}_2] \text{Cl} \text{H}_2\text{O}$
  - (iii)  $\text{Cr}(\text{acac})_3$

- (c) (i) Purification of inorganic complexes using techniques such as crystallisation, volatilisation etc.
- (ii) Tests for purity-M.P., TLC, Metal analysis etc.
- (d) Preparation and study of cis and trans isomers of bis (glycinato) copper(II)
  - (i) Cis-glycinato Cu(II) monohydrate
  - (ii) trans-glycinato Cu(II) monohydrate (IR spectroscopy)
- (e) Preparation of mercury tetrathiocyanato cobaltate :  $\text{Hg}[\text{Co}(\text{CNS})_4]$

#### IV Flame Photometric Determinations

- (a) Sodium and Potassium when present together
- (b) Li/Ca/Ba/Sr Nephelometric determinations
- (a) Sulphate (b) Phosphate (c) Silver

#### V Determination of

- (a) Manganese/Chromium/Vanadium in steel sample by spectrophotometric method
- (b) Ni/Mo/W/V/U by extractive spectrophotometric method.<sub>3</sub>

**Chemistry**  
**M.Sc. Semester-IV**  
**Organic**  
**EC(P)-5**

**Full Marks: 100**  
**Time : 06 Hrs**

**Credit : 5**

**I Organic Synthesis and Extraction of Organic Compounds from Natural Sources**

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

1. Extraction of Caffeine from Tea Leaves (Ref. Experimental Organic Chemistry H Dupon Durst. George W.Gokel, p.464 McGraw Hall Book Co., New York).  
Student should be asked to purify the crude sample, check the purity on a TLC single spot and/or get the pmr scanned and interpret. (Three methyl singlets and 1 methine singlet).
2. Isolation of casein from milk (Try some typical colour reactions of proteins).
3. Isolation of lactose from milk (check purity of sugar by TLC and PC and calculate R<sub>f</sub> value).
4. Isolation of nicotine dipicrate from tobacco.
5. Synthesis of 3-nitrobenzoic acid from benzoic acid.(Ref.: ibid,p. 246-247 and 443-448)  
Aim To demonstrate the process of metanitation, esterification and saponification of an ester.  
Make a comparative study of IR and PMR spectra of benzoic acid, methyl benzoate, methyl 3-nitrobenzoate, if possible.
6. Preparation of Indigo from anthranilic acid
7. Cannizzaro reaction of 4-chlorobenzaldehyde (Ref: ibid, p.397-400).  
Aim To demonstrate technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer.  
Make a comparative study of IR PMR spectra of 4-Chlorobenzyl alcohol if possible.
8. Synthesis of benzanilide from benzene (Ref: ibid, p.775, 812)  
Aim To carry out Friedel Crafts acylation (anhydrous conditions) and Beckman rearrangement. Make a comparative study of the IR and PMR spectra of benzene,

benzophenone, benzophenone oxime and benzanilide (N-H stretching vibrations typical of a secondary amide) if possible.

**II** Characterization of organic compounds. The students is expected to carry out analysis of the components of binary organic mixture (liquid-liquid, liquid-solid and solid-solid). Using chemical analysis and/or IR, and PMR data. The student should also check the purity of the separated components on TLC plates.

**III Quantative 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  $\text{Na}_2\text{CO}_3$ - $\text{KNO}_3$  fusion method.
5. To estimate sulphur in the given sample by Messenger's method.
6. To estimate a halogen in the given sample by the alkaline reduction method (modified Stepanow method).
7. To determine the percentage or number of hydroxyl groups in the given sample by the acetylation method.

**Chemistry**  
**M.Sc. Semester-IV**  
**In-Organic**  
**EC(P)-5**

**Full Marks: 100**

**Time : 06 Hrs**

**Credit : 5**

**I Chemical Kinetics**

1. To study the kinetics of alkaline hydrolysis of an ester in aquo-organic solvent system with respect to effect of solvent composition and dielectric constant on rate constant.
2. To determine the rate constant of the reaction between  $K_2S_2O_8$  and KI at two different temp. and hence to determine the energy of activation of the reaction.

**II. Thermochemistry**

1. Determination of basicity of a polybasic acid.
2. Determination of heat of displacement of Cu by Zn from  $Cu^{2+}$  salt solution.
3. Determination of heat of hydration of  $Na_2SO_4$  to  $Na_2SO_4 \cdot 10 H_2O$ .

**III. Distribution law**

1. Determination of Composition of Cupric-ammine sulphate formed between  $CuSO_4$  and  $NH_3$
2. Determination of equilibrium constant for the reaction  $KI + I_2 = KI_3$

**IV. Thermodynamics and Surface Chemistry**

1. To study the adsorption of acetic acid on charcoal
2. To determine the partial molar volume of solutions of simple salts and to study its variation with concentration

**V. Viscosity and Surface Tension**

1. To determine the radius of a molecule from viscosity measurement.
2. To determine the parachor of  $-CH_2$ , C and H

**Chemistry**  
**M.Sc. Semester-IV**  
**Project**

**Full Marks: 100**

**Time: 06 Hrs**

**Credit: 5**

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 P.G. Department of Chemistry, Nilamber-Pitamber University, Medininagar & open 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 of M.Sc. IV Semester

- (a) Environmental study such as Analysis of water, soil, air etc.
- (b) Industrial goods analysis such as
  - (i) Analysis of Cement
  - (ii) Analysis of minerals available in Jharkhand State
  - (iii) Synthesis of useful commercial products based on raw materials available in Jharkhand state such as Lac, lime-stone etc.
  - (iv) Isolation of Constituents of medicinal plants available Jharkhand State.

Each student has to submit two copies of the dissertation work duly forwarded by the HOD of Department concerned. The forwarded copies will be submitted in the Department of Chemistry, Ranchi University, for evaluation (Seven days before the seminar).

**NB:** The seminar (read the syllabus) will be held in the Deptt. of Chemistry Nilamber-Pitamber University, Medininagar.