# **SYLLABUS**

## M. Sc. CHEMISTRY

## SEMESTER EXAMINATION



## 2019-20

## **DEPARTMENT OF CHEMISTRY**

GOVT. NAGARJUNA POST GRADUATE(AUTONOMOUS) COLLEGE OF SCIENCE, RAIPUR (C.G.)

## SEMESTER STRUCTURE SYSTEM OF M. Sc. CHEMISTRY

- M.Sc. Chemistry has been divided into four Semester comprising of 2400 marks (600 x 4).
- Each semester comprises of four theory papers and two practical's of 600 marks.
- The assessment of each semester is carried by having four theory papers of 80 marks each and internal assessment of 20 marks each.
- The internal assessment of 20 marks/ paper is basically gross evaluation of two unit test per paper of 20 marks each. This marking assessment is applicable only for semester I & semester III.
- For semester II & semester IV 20 marks will be judged by carrying out one seminar per paper.
- There will be Practical exam for selected two papers out of four paper in each semester comprising 100 marks each.

## **Program Specific Outcomes (PSOs)**

- Every branch of Science and technology is inter-related to Chemistry.
- Students understand the major concepts of all discipline of chemistry.
- By means of chemical analysis and experimentation the scope of chemistry can be evaluated in our surroundings. Practically we can ascertain the role of chemistry in physiochemical process to assess the quality of living being.
- In-depth knowledge helps to qualify in various competitive exams.

## **Program Outcomes**

After Completing M.Sc. in Chemistry the following skills can be developed in the students:

- After M.Sc. students can look for the opportunities in R&D department.
- The scientific temperament will be developed in students.
- They understand the qualitative, quantitative methods of analyzing some of the inorganic, organic compounds.
- The use of some of the recent analytical/ instrumental techniques like NMR. XRD, UV-Vis., Chromatography, PES, ESR etc. to evaluate the structural, physical and chemical properties of chemical compounds.
- They can go various industries e.g. dye industry, pharmaceutical, CIPET, mining industry etc.
- They can go for academic field.
- They will get to know the various application of chemical compounds in day to day life.
- They will understand the kinetics, thermodynamics, electrochemical approaches/ changes behind a chemical reaction.

## Ph.D. Program:

- A Ph.D. student will be able to analyze a problem scientifically.
- They will be capable to develop/ modified a method/technique to analyze the data.
- The student can go to various scientific firms like CSIR, ONGC, DRDO, NTPC, UGC etc.
- They can go for higher studies in research institution or go to academic field.

## Course Outcomes

## M.Sc. Outcome:

- A good knowledge about the basic concept and application of polymer chemistry, quantum chemistry, thermodynamics, nuclear chemistry.
- The preparation, properties and applications of co-ordination and organometallic compounds.
- The understanding of how a drug is designed, the steps involved in designing a drug how does it work in the body.
- The understanding of cause of environmental pollution and methods & techniques apply to control it.
- Analytical chemistry gives good perspectives of the theories and understanding of different errors, methods for minimizing errors.
- Single and multistep synthesis of some organic compounds and its derivative.
- Students will able for estimate the functional group, extraction of organic compounds from natural sources.

### **EXAMINATION SCHEME**

# M.Sc. examination will be conducted in four SEMESTERS. Each semester exam shall consist of FOUR THEORY PAPERS and TWO LAB Courses.

### **SEMESTER-I**

## **DISTRIBUTION OF MARKS**

## **SEMESTER –I (20 CREDIT)**

## **THEORY (16 CREDIT)**

No	Nome of Paper		Marks		Credit Points
110.	Name of Faper	Theory	Internal assessment ( Unit Test)	Total Marks	
Ι	Inorganic Chemistry	80	20	100	04
II	Organic Chemistry	80	20	100	04
III	Physical Chemistry	80	20	100	04
IV	Basics Of Spectroscopy	80	20	100	04

## **PRACTICAL (4 CREDIT)**

Course	Paper	Marks	Two Experiment	Viva	Sessional	Credit	Time
Practical-1	Inorganic Chemistry	100	60	20	20	02	10 Hr
Practical-2	Physical Chemistry	100	60	20	20	02	6 Hr

### SEMESTER – I Paper- I Inorganic Chemistry

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	<b>MM 80</b>

### Unit-I

**Symmetry and Group Theory in Chemistry:** 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. Schoenflies symbols, representations 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 and their use in spectroscopy.

### Unit-II

The Structure and Reactivity of Molecules: VSEPR theory (Sidgwick, Powel & Gillespie and Nyholm theory) Walsh diagrams (tri & penta atomic molecules), hybridization, Bent rule and energetic of hybridization, non bonded repulsions, Bent bonds,  $d\pi$ -  $P\pi$  bonds, bond length and bond multiplicity. Physical method of determination of molecular structure. Some simple reactions of covalently bonded molecules, atomic inversion, berry pseudo rotation, Nucleophilic displacement, free radical mechanisms.

### Unit-III

**Structure and Stereoisomerism in Co-ordination Compounds:** Geometrical and optical isomerism in 4 and 6 coordination compounds, resolution of racemic mixture. Molecular rearrangement in 4 and 6 coordination compounds. Stereochemistry of complexes having coordination number 3, 5, 7 and 8. Methods used for their characterization. Effect of non bonding electrons on the preferred stereochemistry of Transition metal complexes exhibiting the coordination number 3, 5, 7 and 8.

### **Unit-IV**

**Metal-Ligand Equilibria in Solution:** Stepwise and overall formation constant and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion & ligand, crystal field effect and natural order of stability,

chelate effect and its thermodynamic origin. Determination of binary formation constant by spectrophotometry (absorbance method, Jobs, method, limiting logarithmic method, and mole ratio method) and potentiometric method.

**Metal – Ligand Bonding:** Crystal field theory, distortion octahedral complexes and John Teller theorem, CFSE and its uses, limitation of crystal field theory, experimental evidences for metalligand covalent bonding in complexes, molecular orbital theory, MOT for octahedral complexes with and without bonding, MOT for tetrahedral and square planar complexes with and without bonding. Effect of bonding on the value of  $\Delta_{o}$ , relation between bonding ability and spectrochemical series.

### **Books Suggested:**

1. Advanced Inorganic Chemistry. F. A. Cotton and Wilkinson, John.

- 2.Inorganic Chemistry J. E. Huhey, Harpes & Row.
- 3. Chemistry of the Elements N. N. Greenwood & A. Earnshow, Pergamon.

4.Compherensive co-ordination Chemistry by G. Wilkinson, R.D. Gallares & J. A. Mcclevetty Pergamoil.

5.Co-ordination Chemistry, S,S. Rao and Vani Rao, Kalyani Publishers

7 Symmetry and Group Theory, Veera Reddy

8. Inorganic electronic spectroscopy, A.B.P. Lever, Elsevier

### **SEMESTER-I**

### Paper –II

### **Organic Chemistry**

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT) .	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT)	internal
	MM 80

### Unit –I

**Nature of Bonding in Organic Molecules:** Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non – benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of - molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, cyclodextrins, catenanes and rotaxanes.

**Reaction Intermediates: Structural Reactivity:** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity – resonance and field effects, quantitative treatement, the Hammett equation and linear free energy relation ship, substituent and reaction constant Taft equation.

### Unit- II

**Reaction Mechanism:** Types of mechanism, 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

Aliphatic Nucleophilic Substitution: The  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^1 \& S_N^2$  and SET mechanisms The neighboring group mechanism, neighboring group participation by  $\sigma$ - and  $\pi$ - bonds. Anchimeric assistance.

Aromatic Nucleophilic Substitution: The  $S_NAr$ ,  $S_N^{1}$ , benzyne and  $S_{RN}^{1}$  mechanism, reactivity: effect of substrate structure, leaving group and attacking nucleophiles. The von-Richter, Sommelet–Hauser and Smiles rearrangements.

### Unit III

Aliphatic Electrophilic Substitutions: Bimolecular mechanism:  $S_E^2 \& S_E^{-1}$ . The  $S_E^{-1}$  mechanism, electrophilic substitution accompanied bydouble bond shifts, effect of substrate, leaving group and the solvent polarity on the reactivity.

**Aromatic Electrophilic Substitution:** 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. Vilsmeir reaction, Gattermann – Koch reaction.

### Unit IV

**Stereochemistry:** Conformational analysis of cycloalkanes, decalines, effects of conformation on reactivity. Conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diasterotopic atoms, groups and faces. Stereo specific & stereo selective synthesis. Asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes). Chirality due to spherical shape.

### **Books Suggested:**

1. Advanced General Organic Chemistry, Sachin Kumar Ghosh.

2.Organic Reactions and their mechanism, P. S. Kalsi.

3. Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March.

4. Advanced Organic Chemistry, F.A. Careu and R.J. Sunberg..

5.A Guidebook of mechanism in Organic Chemistry, C. K. Ingold.

6.Organic Chemistry, R.T. Morrison and R. N. Boyd.

7. Structure and Mechanism in Organic Chemistry, Peter Skyes.

8. Modern Organic Reactions, Benzamine.

9. Stereochemistry of Organic Compounds, D. Nasipuri.

10. Stereochemistry of Organic Compounds, P. S. Kalsi.

#### **SEMESTER –I**

#### Paper-III

### **Physical Chemistry**

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

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Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	MM 80

### Unit I

**Differential Calculus:** Functions: continuity and differentiability. Rules for differentiation. Application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels. Bohr's radius and most probable velocity from Maxwell's distribution etc-, exact and inexact differential with their applications to thermodynamic properties) Integral calculus, basic rules for integration, integration by parts. Partial fraction and substitution, reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar), curve sketching.

**Elementary Differential Equations:** Variables- separable and exact first order differential equations, homogeneous. Exact and liner equations, application to chemical kinetics secular equilibria quantum chemistry etc. second order differential equations and their solutions.

**Permutation & probability:** Permutation & combinations, probability & probability theorems, probability curves. Examples from kinetic theory of gases etc.

### Unit--II

**Introduction to Exact Quantum Mechanical Rules:** The Schrödinger equation and postulates of quantum mechanics. Discussion of solutions of Schrödinger equation to some model systems viz. Particle in a box.

**Approximation Methods:** Harmonic oscillator, the rigid rotator, The hydrogen atom. The variation theorem and linear variation principles. Perturbation theory (first order and non-degenerate) Applications of variation method and perturbation theory to the helium atoms.

**Angular Momentum:** Ordinary angular momentum generalized angular momentum, eigen functions for angular momentum, eigen value angular momentum, operator using ladder operators, addition of angular momentum, spin, anti-symmetry & pauli's exclusions principles.

### Unit-III

Electronic States of Atoms: Electronic configuration, Russel-Saunder terms and coupling constant, Slater-condon parameters, Term separation energies of the  $p^n$  configuration, term separation energies for the  $d^n$  configuration, magnetic effects, spin orbit coupling, Zeeman effect splitting, introduction to the methods of self-consistent field, the viral theorem.

**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 Huckel theory.

### Unit-IV

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

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

### **Books Suggested:-**

1. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.

2. Chemical Mathematics, D. M. Hirst, Longman.

- 3.Basic Mathematics for Chemists, Tebbutt, Wiley.
- 4. Mathematics for Chemists, Niranjan and Tripathi, Anusandhan Prakashan.
- 5. Introduction to Quantum Chemistry, A. K. Chandra, Tata Mcgraw Hill.
- 6. Quantum Chemistry, B. K. Sen.
- 7. Quantum Chemistry, Ira and Levine, Prentice Hall.
- 8. Physical Chemistry, P.W. Atkins, Elbs.
- 9. Chemical Kinetics, K. J. Laidler, Mcgraw Hill.

### Semester –I

### **Paper-IV**

### **Basics Of Spectroscopy**

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	<b>MM 80</b>

### Unit-I

**Unifying Principles:** Electromagnetic radiation, interaction of electromagnetic radiation with matter ,absorption, emission, transmission, reflection, dispersion, polarization and scattering. Uncertainty relation & 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 & electronic energy levels.

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

### Unit-II

Atomic Spectroscopy: Energies of atomic orbitals, vector representation of momenta and vector coupling spectra of hydrogen atom and alkali metal atoms. Basic features of spectrometers, Width and intensity of spectral lines, selection rules for atomic spectra.

**UV-Visible Spectroscopy :** Introduction, Theory of UV-visible spectrometer, Beer's Lambert's Law, Bathochromic Shift, Hypsochromic Shift, Hyper and Hypo chromic Shift, Colour of compounds, Auxochrome, types of transition in organic molecules, Solvent effect on electronic transition, selection rule for electronic transition, Woodward-Fieser rule for polyenes and  $\alpha$ - $\beta$  unsaturated carbonyl compounds, application of UV-visible spectroscopy

## Unit-III

**Molecular Spectroscopy:** Energy levels, molecular orbital, vibronic transitions, vibrational progressions and geometry of the excited states, Frank - Condon principle, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion, inter system crossing, Kasha's rule, Jablonski diagram and spectra of transition metal complexes, charge- transfers spectra.

**Photoelectron Spectroscopy:** Basic principles, photo- electric effect, ionization process, Koopman's theorem, Photoelectron spectra of simple molecules. ESCA, chemical information from ESCA. Auger electron spectroscopy –basic idea.

### Unit-IV

**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

**Raman Spectroscopy:** Classical and quantum theories of Raman effect, Pure rotational, vibrational and vibrational - rotational Raman spectra, selection rules, mutual exclusion principles. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

### **Books Suggested:-**

1. Modern Spectroscopy J. M. Hollas, John Willey.

2.Applied Electron Spectroscopy for chemical analysis Ed. H. Windawi and F. I. Willey Interscience.

3. Spectroscopy, H. Kaur, Pragati, Prakashan

4. Molecular Spectroscopy, Banwall.

5. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.

6.Molecular Spectroscopy, P. S. Sindhu, New Age International.

7.An Introduction to Spectroscopy, S. S. Kalra, Anusandhan Prakashan

8. Group Theory by Cotton& Wilkinson.

9. Group Theory, Bhattacharya, Goel Publisher.

10. Molecular Symmetry and its application, Shukla and Kumar, Anusandhan Prakashan.

## SEMESTER – I

### **LABORATORY COURSE - 01**

### **Inorganic Chemistry**

### Time-10 Hrs

### MM 100

### **Quantitative analysis**

Separation and determination of two metal ions from solution mixtures. One by Volumetric and other by Gravimetric methods Cu-Ni, Ni-Zn,Cu-Fe etc

## Preparation of selected inorganic compounds.

- cis-K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]
- [Mn (acac)<sub>3</sub>]
- $K_3[Fe(C_2O_4)_3]$
- Prussian blue, Turnbull's blue
- $[Ni (NH_3)_6]Cl_2$
- [Ni (dmg) <sub>2</sub>]
- [Cu (NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>O

Qualitative analysis of mixture containing 08 radicals including two less common metal ions by semi micro method

**Basic radicals:**  $Ag^{I}$ ,  $Pb^{II}$ ,  $Bi^{III}$ ,  $Cu^{II}$ ,  $Cd^{II}$ ,  $As^{III}$ ,  $Sb^{III}$ ,  $Sn^{II}$ ,  $Fe^{III}$ ,  $Al^{III}$ ,  $Cr^{III}$ ,  $Zn^{II}$ ,  $Mn^{II}$ ,  $Co^{II}$ ,  $Ni^{II}$ ,  $Ba^{II}$ ,  $Ca^{II}$ ,  $Mg^{II}$ ,  $Na^{I}$ ,  $K^{I}$ ,  $Ce^{IV}$ ,  $Th^{IV}$ ,  $Zr^{IV}$ ,  $W^{VI}$ ,  $Te^{IV}$ ,  $Ti^{I}$ ,  $Mo^{VI}$ ,  $U^{VI}$ ,  $V^{V}$ ,  $Be^{II}$ ,  $Li^{I}$ ,  $Au^{I}$ ,  $Pt^{IV}$ ,

Acid radicals: Carbonate, sulphide, sulphate, nitrite, nitrate, acetate, chloride, fluoride,Bromide, iodide, borate, sulphonate, oxalate, phosphate, silicate, thiosulphate,Ferrocyanide, ferricyanide, sulphocyanide, chromate, arsenate and permanganate

### Estimation

- Phosphoric acid in commercial ortho- phosphoric acid.
- Boric acid in borax.
- Ammonia in ammonium salt.
- Manganese dioxide in pyrolusite.
- Available chlorine in bleaching powder.
- Hydrogen per oxide commercial sample.

### Note:- Two exercises will be given to students in the practical examination of 10 hrs duration

## SEMESTER –I LABORATORY COURSE - 02

## **Physical Chemistry Practical**

## **Time-06 Hrs**

### Adsorption

To verify the freundlich and Longmuir isotherms for adsorption of acetic acid on activated charcoal.

To study adsorption of oxalic acid on charcoal using KMnO<sub>4</sub>

To study adsorption of picric acid on charcoal by colorimeter.

## Polarimetry

Study the kinetics of hydrolysis of cane sugar

Determination of catalytic coefficient of hydronium ion catalyst (Inversion of sugar at low acid concentration)

Determination of specific rotation of glucose and fructose solution

Determination of velocity constant of the inversion of sugar by mono, di and trichloro acetic acid.

## **Chemical Kinetics**

Determination of effect of temperature, change of concentration of reactants and catalyst and ionic strength of the media on the velocity constant of hydrolysis of an ester /ionic reactions Determination of velocity constant of the hydrolysis of an ester in micellar media.

Determination of rate constant of oxidation of iodide ions by hydrogen peroxide by studying the Kinetics as an iodine clock reaction.

### Solutions

To determine the critical micelle concentration of a soap (Sodium laurate, Sodium palmilate etc.) by surface tension measurements.

To compare cleaning powders of two samples of detergent.

Determine the critical solution temperature of phenol and water in presence of (I) 1.0% sodium chloride (II) 0.50 % naphthalene (III) 1.0% Succinic acid.

## Electrochemistry

## Conductometry

Determination of velocity constant, order of reaction and energy of activation for saponofication of ethyl acetate by NaOH conducto metrically.

Determination of solubility and solubility product of sparingly soluble salts (PbSO<sub>4</sub>, BaSO<sub>4</sub>)

Conducto-metrically

Determination of strong and weak acids in a given mixture conducto-metrically.

Determination of the activity coefficient of HCl at different concentrations using

Debye-Huckel's law.

## **Potentiometry / pH metry**

Determination of strength of strong and weak acids in a given mixture using potentiometer /pH meter.

Determination of temperature dependence of EMF of a cell.

Acid base titration in aqueous media using a pH meter.

Determination of activity and activity coefficient of electrolytes

Determination of dissociation constant of mono-basic/di-basic acid.

Construct the calibration curve ( pH-Eobs ) for quinhydrone electrode, and hence determine the standard oxidation potential of the quinhydrone electrode

## **Reference Books :**

Advance Practical Physical Chemistry- Dr. J.B. Yadav Krishna Prakashan Media(P) LTd, Merut. Senior Practical Physical Chemistry Dr. B.D. Khosla, V.C. Garg, Adarsh Gulani- R.Chand & W New Delhi.

Experiments in Physical Chemistry by Dr. J.C. Ghosh- Bharati Bhawan.

## **SEMESTER –III (20 CREDIT)**

## DISTRIBUTION OF MARKS IN THEORY AND PRACTICAL

## **THEORY (16 CREDIT)**

NT	N		Marks		
<b>NO.</b>	Name of Paper	Theory	Internal assessment ( Unit Test)	Total Marks	Points
Ι	Organo-transition metal Chemistry	80	20	100	04
Π	Natural Product	80	20	100	04
III	Solid state and Polymer Chemistry	80	20	100	04
IV	Environmental and Analytical Chemistry	80	20	100	04

## **PRACTICAL (4 CREDIT)**

Course	Paper	Marks	Two Experiment	Viva	Sessional	Credit	Time
Practical-1	Organic Chemistry	100	60	20	20	02	8 Hr
Practical-2	Analytical Chemistry	100	60	20	20	02	8 Hr

### **SEMESTER-III**

### Paper-I

### **Organo-transition Metal Chemistry**

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT) .	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	MM 80

### Unit-I

**Alkyls and Aryls of Transition Metals:** -Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

**Compounds of Transition Metal-Carbon Multiple Bonds:** - Alkylidenes, alkylidynes, low valent carbenes and carbines-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

### Unit-II

**Transition Metal**  $\pi$ - **Complexes:** - Transition metal  $\pi$ -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complex, preparations, properties, nature of bonding and structure features. Important reactions relating to nucleophilic and electrophilic attack on ligands and organic synthesis.

### Unit-III

**Homogenous Catalysis:** - Stoichiometric reactions for catalysis, homogenous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalysis reactions involving carbon mono oxide such as hydrocarbonylation of olefins, (oxo reaction), Oxo palladation reactions, activation of C-H bond.

### **Unit-IV**

**Transition Metals Compound With Bond to Hydrogen: -** Transition metal compounds with bonds to hydrogen.

**Fluxional Organometallic Compounds:** - Fluxionality and dynamic equillibria in compounds such as  $n^2$  - olefin,  $n^3$  -allyl and dienyl complexes.

## **Book Suggested: -**

1. Principles and Application of Organotransition Metal Chemistry J.P. Colliman, L.S.

Hegsdus, J.R. Norton and R.G. Finke, University Science Books.

2. The Organometallic Chemistry of —The Transition Metals, Rh Crabtree, John Wiley.

3. Metallo-Organic Chemistry, A.J. Pearson, Wiley.

4.Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

### **SEMESTER-III**

### Paper-II

### **Natural Products**

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

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Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT)	internal
	<b>MM 80</b>

### Unit-I

**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 and synthesisof Ephedrine, Coniine(+\_), Nicotine, Quinine, Atropine and Morphine.

### Unit-II

**Terpenoids and Carotenoids:** -Classification, nomenclature, occurrence, isolation, general methods of determination of Citral, Geraniol,  $\alpha$ -Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and  $\beta$ -Carotene.

### Unit-III

**Steroids and Hormones:** - Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and biosynthesis of Cholesterol.

### Unit-IV

Plant Pigments: Classification, Flavones, Flavonols and Isoflavones, structure and synthesis of Luteolin, Apigenin, Quercetin, Myricitin, Diadzein and Genistein, biosynthesis of Flavonols.
Anthocyanins: - General methods for structure determination, structure and synthesis of Cyanidin, Pelargonidin, Delphinidin, Malvidin and Hirsutidin.

**Pyrrole Pigments: -** Porphyrines, structure and synthesis of Haemoglobin and ChlorophyllRelationship between Haemoglobin and Chlorophyll.

### **Book Suggested: -**

1. Organic Chemistry, D.V. Banthrope, Longman Essex, J. B. Harbrone.

2.Streoselective Synthesis, M. Nogradi and CHV. Odds

3. Chemistry of Carbon Compounds, ED.S. Coffey, Elsevier.

4. Biological and Pharmacological Properties of Medicinal Plants from Americans, M. P. Gupta

and A. Marston, Harwood Academic Publishers.

5. Insecticides of Natural Origin, Sukh Dev.

6.An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock.

7.Berger's Medicinal Chemistry and Drug Discovery, Vol-i (Chapter-9 and Ch-14). Goodman and Gillman's Pharmacological Basis of Therapeutics, Mc Graw Hill.

### **SEMESTER –III**

### **Paper-III**

### **Solid State and Polymers**

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) from all FOUR unit.

Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) with internal choices (06 marks for each UNIT).

Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) internal with choice (12 marks for each UNIT).

**MM 80** 

### Unit-I

**Crystal Defects and Non-Stoichiometry: -** Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defects formation, colour centers, non-stoichiometry and defects.

**Electronic Properties and Band Theory:** - Metals, insulator and semiconductors, electronic, structure of solids-band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semi conductors, doping conductors, p-n junctions, super conductors, optical properties- optical reflectance, photoconduction photoelectric effects.

### Unit-II

**Magnetic Properties-** Classification of materials, Quantum theory of paramagnetic cooperative phenomena magnetic domains, hysteresius.

**Organic Solids:** - Electrically conducting solids, organic charge transfer complex, organic metals, and new super conductors.

**Solid State Reactions:** - General principles, experimental procedures, co-precipitation as a precursor to solid-state reactions, kinetics of solid-state reactions.

### Unit-III

**Basics and Characterization of Polymers** - Importance of polymers, types of polymers, electrically conducting fire resistant, Mass liquid crystal polymers, Kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods) Sedimentation, chain configuration of macromolecules, calculation of average dimension of macromolecules.

### **Unit-IV**

**Structure and properties of polymers: -**Morphology and order in crystalline polymers, configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain- induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point Tm- melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg – relationship between Tm and Tg, effects of molecular weight, diluents,

chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

### **Book Suggested: -**

1.Solid State Chemistry and its Applications, A.R. West, Plenum.

2. Principle of the Solid State, H.V. Keer, Wiley Eastern.

3. Solis State Chemistry, D.K. Chakrabarty, New Age International.

4. Text book of polymer science, F. W. Billmeyer, Jr. Wiley.

5.Polymer science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Wiley - Eastern.

6. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and Professional.

### **SEMESTER –III**

### Paper-IV

### **Environmental & Analytical Chemistry**

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	<b>MM 80</b>

### Unit-I

**Environment:** - Introduction, composition of atmosphere, vertical temperature Profile, Heat/radiation budget of the earth atmospheric system, vertical stability, atmosphere. Biogeochemical cycles of C, N, P, S, and biodistribution elements.

Atmospheric Chemistry: - 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 polluton 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.

### Unit-II

**Aquatic Chemistry:** -Chemical composition of water bodies-lakes, streams, rivers and wetlands. Hydrological cycle. Aquatic pollution- inorganic, organic, pesticides, industrial, agricultural soil, detergents, oil spills, oil pollutants and radioactive wastes as source of pollution. Water quality parameters - dissolved oxygen, biochemical oxygen demand, chemical oxygen demand, solids, and metals, content of chloride, sulphate, phosphate, nitrate and microorganisms. Water quality standards

**Analysis of Water Pollution:** - Water pollutants and their effects. Sources of water pollution. 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'

### Unit III

**Industrial Pollution:** - Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers, drugs, Radio nuclide analysis, Disposal of wastes and their management.

**Soil and Environmental Disasters: -** Soil composition, micro and macronutrients moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali, salts. Soil pollution by fertilizers, plastics and metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, Three Mile Island Sewozo and Minimata disasters.

## Unit IV

### Analysis of Fuel, Body Fluid and Drugs

**Fuel analysis:** Solids, liquid and gas. Ultimate and proximate analysis heating values grading of cola, liquid, fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels producer gas and water gas calorific value.

**Clinical analysis:** 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 phosphates. Immunoassay, principles of radioimmunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

**Drug analysis**: Narcotics and dangerous drugs, classification of drugs screening by gas and thin layer chromatography and spectrometric measurements.

### **Book Suggested: -**

1. Environmental Chemistry, Samir K. Banerji; Prentice Hall of India.

2. Environmental Chemistry, Sharma & Kaur; Krishna Publishes.

3. Environmental Chemistry, A. K. Dey, Wiley Eastern.

4. Chemistry of Atmosphere, R. P. Wayne; Oxford.

5.A Text Book of Environmental Chemistry and Pollution Control, S. S. Dara; S. Chand Publication.

6. Environmental Solution Analysis, S.M. Khopkar; Wiley Eastern.

- 7. Analytical Chemistry, G. D. Christian; J. Wiley
- 8. Environmental Solution Analysis, S.M. Khopkar; Wiley Eastern.
- 9. Principle of Instrumental Analysis, D. A. Skoog, J. L. Loary and W. B. Saunders
- 10. Basic Concepts of Analytical Chemistry, S.M. Khopkar; Wiley Eastern.
- 11. Analytical Chemistry, B. K. Sharma; Krishna Prakashan Media (P) Ltd. Meerut.

## Semester –III

## **LABORATORY COURSE - 01**

## **Organic Chemistry**

MM 100

## Multi step Synthesis of Organic Compounds

- Beckmann rearrangement: Benzanilide from benzene (Benzene, Benzophenone, Benzophenone oxime ,Benzanilide).
- Benzilic acid rearrangement: Benzilic acid from Benzoin (Benzoin, Benzil, Benzillic acid)
- Skraup's synthesis (Synthises of heterocyclic compounds) Quinoline from o-amino phenol
- m-Nitroaniline from benzene (Benzene, nitrobenzene, m-dinitrobenzene, m-nitroaniline)
- Acridone from anthranilic acid (Anthranilic acid, o-chlorobenzoic acid, N-phenylanthranilic acid, acridone).
- Enzymatic synthesis: Enzymatic reduction: Reduction of ethylacetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ethyl-3–hydroxybutanoate and determine its optical purity. Biosynthesis of ethanol from sucrose.

## **Quantitative Organic Analysis**

- Estimation of sulphur by Messenger's method.
- Estimation of nitrogen by Kjeldahl method.

## **Estimation of Functional Group**

- Estimation of aniline.
- Estimation of amino group by acetylation method.
- Estimation of hydroxyl group by acetylation method.
- Estimation of carbonyl group by hydrazone formation method.
- Estimation of carboxyl group by titration method.
- Determination of equivalent weight of carboxylic acid by silver salt method.
- Estimation of glucose by Fehling solution method.
- Estimation of glycine by titration method.

## **Extraction of Organic Compounds from Natural Sources**

- Isolation of caffine from tea leaves.
- Isolation of casein from milk: perform colour reaction of protein.
- Isolation of lactose from milk: purity of sugar should be checked by TLC and PC and Rf value reported.
- Isolation of nicotine dipicrate from tobacco.

- Isolation of cinchonine from cinchona bark.
- Isolation of piperine from black pepper.
- Isolation of lycopene from tomatoes.
- Isolation of  $\beta$ -carotene from carrots.
- Isolation of limonene from citrus rinds.
- Isolation of protein and carbohydrates from seeds colour test.
- Extraction of fatty oil from seeds and determination of refractive index of the oil.
- Isolation of protein and carbohydrate (as reducing sugars) from seed-colour test.

## **Books Suggested:**

- Practical organic chemistry by A. I. Vogel.
- Practical organic chemistry by Mann and Saunders.
- Practical organic chemistry by Garg and Saluja.
- The systematic identification of Organic compounds, R.L. Shriner and D.Y. Curtin.

## SEMESTER –III LABORATORY COURSE – 02

## **Analytical Chemistry**

**MM 100** 

## **Phase Equilibrium:**

- Determination of triangular phase diagram of acetic acid, chloroform and water.
- Determination of phase diagrams for acetone, ester and water system.
- Determination of triangular phase diagram of acetic acid, chloroform and water.
- Determination of triangular phase diagram of phosphoric acid, ester and water.
- Determination of triangular phase diagram of ethanol, benzene, and water system
- Determination of triangular phase diagram of benzene, acetic acid and water system
- Determination of distribution coefficient of succinic acid between ether and water.
- Determination of the formula of the complex formed between the cupric ion and ammonia by distribution method.

### Spectroscopy

- Determination of stoichiometry and stability constant of complexes (ferric-salicylic acid and amine iodine complex.
- Interpretation of spectra (UV, NMR, Mass etc.) of organic/ inorganic compounds.

## **Spectrophotometric Determination:**

- Determination of metal ions e.g. Fe, Cu, Zn, Pb, etc. using inorganic reagent like SCN<sup>-</sup> and organic chelating agent like dithiazone, cupferon, 8-hydroxyquinoline, etc in aqueous / organic phase in the presence of surface active agents.
- Mn, Cr and V in steel sample.
- Ni, Mo, W, V and U by extractive spectrophotometric method.
- Fe- phenonthrolein complex, Jobs' method of continuous variation.
- Cu-ethylene diamines by slope ratio method.
- Determination of Phosphate concentration in soft drinks
- Determination of strength of base
- Determination of dissociation constant of some acid -base indicator
- Phosphate determination
- Sulphate determination
- $\lambda_{max}$  determination

## pH – Metry

- Effect of pH in aqueous colored system.
- Stepwise proton ligand and metal ligand stability constant of complex by Leaving-

## Nephelometric / Turbidimetric Determination

1. Sulphate 2. Phosphate 3. Silver

## **EMF of Cells**

- Determination of ionic products of water by EMF method
- Determination of pH of mixture of CH<sub>3</sub>COOH & CH<sub>3</sub>COONa and dissociation constant of the acids
- Determination of pH of solution by glass electrode.

## **Titrimetric / Gravimetric Determinations**

- Mn in steel/ Iron by Bismuthal/ / Iodate method.
- Mn in Pyrolusite ore.
- Ni in steel by DMG method.
- Pb by Dithiozone precipitation method.
- Chromium in chromite ore.
- Fluoride in water.

## **SEMESTER –II (20 CREDIT)**

## **DISTRIBUTION OF MARKS**

## **THEORY (16 CREDITS)**

No.	Name of Paper					
		Theory	Internal assessment	Total Marks	Points	
			( Unit Test)			
Ι	Co-ordination Chemistry	80	20	100	04	
II	Organic Chemistry	80	20	100	04	
III	Physical Chemistry	80	20	100	04	
IV	Spectroscopy & Computer for Chemist	80	20	100	04	

## PRACTICAL (4 CREDIT)

Course	Paper	Marks	Two Experiment	Viva	Sessional	Credit	Time
Practical-1	Organic Chemistry	100	60	20	20	02	6 Hr
Practical-2	Analytical Chemistry	100	60	20	20	02	6 Hr

### Semester-II Paper I Coordination Chemistry

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT) .	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT)	internal
	<b>MM 80</b>

### Unit I

**Reaction Mechanisms of Transition Metal Complexes Part I**: Rate of reaction, the rate law, effective collision, Energy profile of reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, classification of mechanism of ligand substitution, kinetics and mechanisms of octahedral substitution, hydrolysis reaction, acid hydrolysis reaction in octahedral complexes with and without  $\pi$  bonding inert ligands, factors affecting acid hydrolysis reaction, base hydrolysis reaction, conjugate base mechanism, direct & indirect evidences in favor of conjugate base mechanism, Kinetics and mechanisms of anation reactions, kinetics of acid catalyzed reaction, kinetics of reaction without metal-ligand bond cleavage.

### Unit II

**Reaction Mechanism of Transition Metal Complexes Part II**: Kinetics and mechanisms ligand substitution reaction in square planner complexes, factors affecting the mechanism of square planner complexes. The Trans effect: theories and applications. Kinetics of ligand substitution reaction in tetrahedral complexes. Redox reactions, electron transfer reaction, mechanism of one – electron transfer reaction, outer sphere type reaction, Marcus theory, simplified Marcus equation, excited state outer sphere electron transfer reaction, cross reaction, inner sphere reactions, types, mechanisms electron transfer in inner sphere reaction, mechanism of two electron transfer.

### **Unit-III**

Electronic Spectra and Magnetic Properties of Transition Metal Complexes: Determination of spectroscopic ground states, Hunds rule, term symbols for excited states, microstates and derivation of Russell – saunders terms, Selection rule for electronic spectroscopy, correlation, orgel and Tanabe –Sugano diagrams for transition complexes ( $d^1-d^9$  states). Nephelauxetic effect, calculations of Dq and B and B<sup>c</sup> parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, quenching of orbital angular momentum, orbital contribution to magnetic moment, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

### Unit-IV

**Metal Clusters:** Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Metal  $\pi$  Complexes: Metal carbonyl, 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.

### **Books Suggested**

1. Advanced Inorganic Chemistry, F.A. Cotton John Wieley.

- 2.Inorganic Chemistry, J.E. Huheey Harper & Row.
- 3.Co-ordination Chemistry; D. Banerjea, Asian Books PVT. LTD.
- 4. Magneto Chemistry, Shyamal Dutta.
- 5.Co-ordination Chemistry, S,S. Rao and Vani Rao, Kalyani Publishers
- 6. Advanced Inorganic Chemistry, Keemti Lal and Agrawala, Pragati Prakashan.
- 7. Inorganic Chemistry Part I & II, Rashmi Jain, Usha Soni, Pragati Prakashan.

### SEMESTER-II Paper- II Organic Chemistry QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) from all FOUR unit.

Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) with internal choices (06 marks for each UNIT).

Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) internal with choice (12 marks for each UNIT).

## **MM 80**

### Unit-1

**Free Radical Reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at aromatic substrate, neighboring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents reactivity. Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sanmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**Elimination Reactions:** The E1, E2, and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity -effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

### Unit- II

Addition to Carbon – Carbon Multiple Bonds: Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals regio and chemo selectivity, orientation and reactivity. Addition to cyclopropane ring, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, sharpless asymmetric epoxidation.

### Unit-III

Addition to Carbon – Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction. Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, amminolysis of esters.

### **Unit-IV**

**Pericyclic Reactions:** Molecular orbital, symmetry, frontier orbitals of ethylene, 1, 3-Butadiene, 1, 3, 5 –hexatriene and allyl system. Classification of Pericyclic reactions, Woodward – Hoffmann correlation diagrams. FMO & PMO approach. Electrocyclic reactions conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems Cycloadditions-antarafacial and suprafacial addition, 4n and 4n + 2 systems, 2+2 addition of ketenes, 1,3 dipolar cyclo additions and cheleotopic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3 and 5, 5 sigmatropic rearrangements Claisen, Cope and Aza - Cope rearrangements, Fluxional tautomerism Ene reaction.

### **Books Suggested:-**

1Advanced organic chemistry - reactions, mechanism & structure, Jerry March

2.Advanced organic chemistry, F.A. Careu & R. J. Sunberg Plenum.

3.A Guide book of mechanism in organic chemistry, C. K. Ingold, Cornell Univ. Press.

4.Organic chemistry, R. T. Morrison & R. N. Boyd, Prentice Hall.

5.Structure & mechanism in organic chemistry, Peter Skyes, Longman.

6.Modern organic reactions, H. O. House, Benjamin.

7. Pericyclic Reactions, S. M. Mukherjee, Macmillan, India.

8. Reaction Mechanism in Organic chemistry S. M. Mukherjee & S. P. Singh.

9. Advanced General Organic Chemistry, Sachin Kumar Ghosh.

10.Organic Reactions and their mechanism, P. S. Kalsi.

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### SEMESTER –II Paper –III Physical Chemistry QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT)	internal
	MM 80

## Unit –I

**Classical Thermodynamics:** 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. Determination of these quantities. Concept of fugacity and determination of fugacity Non- ideal system: Excess functions for non – ideal solutions. Activity and activity coefficient, Debye –Huckel theory for activity coefficient of electrolytic solutions. Determination of activity and activity coefficients, ionic strength. Application of phase rule to three component systems, second order phase transition

## Unit-II

**Statistical Thermodynamics:** Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging canonical, grand canonical and micro Canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions—transnational rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions. Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi – Dirac Statistics , Distribution law and application to metal ,Bose- Einstein Statistics—distribution law and application to Helium.

**Non- Equilibrium Thermodynamic:** Thermodynamics criteria for non equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc. ) transformations of the generalized fluxes and forces , non –equilibrium stationary states, phenomenological equations microscopic reversibility and Onsager's reciprocity relations, electrokinetic's phenomena ,diffusion, electric conduction, irreversible , thermodynamics for biological systems, coupled reactions.

### **Unit-III**

**Electrochemistry:** Electrochemistry of solutions Debye – Huckel theory, mathematical derivation of Debye – Huckel equation. Debye – Huckel - Onsager treatment and its extention. Wien effect, Debye – Falkenhagen effect. Ion solvent interactions - thermodynamics of electrified interfaces equations, Lippmann equations. Structure of electrified interfaces – the parallel plate condenser model (Hemholtz-perrien theory), Guoy – Chapman theory, Stern's theory. Overpotentials (types, measurement, theories, importance and factors affecting overpotentials), exchange current density, derivation of Butler-Volmer equation, Tefel plot. Polarography theory ; Ilkovic equation, half wave potential and its significance. Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention methods.

### Unit-IV

**Electrocatalysis:** Relative power of electrocatalysts, mechanism of electrocatalysis, Volcanoes, Platinum as a catalyst. Bioelectrocatalysis- enzymes and immobilization.

### **Surface Chemistry**

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 film on liquids (Electro kinetic phenomenon), and Catalytic activity at surfaces.

**Micelles:** Surface-active agents, classification of surface-active agents, micellization, hydrophobic interacton, critical micellar concentration (CMC). factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

### **Books Suggested:-**

1. Physical Chemistry, P.W. Atkins, ELBS.

2. Statistical Thermodynamics, Gupta and Kumar.

3. Mechanical Statistics, D. M. Hirst.

4. Modern Electrochemistry Vol. 1 and 2, J.O.M. Bockrisad and A.K.N. Reddy, Plenum.

5. Electrochemistry, L. Andropov.

6.Modern Electrochemistry, Roger Philip.

7. Micelles, Theoretical & applied aspects, V. Mori, Plenum.

### **SEMESTER-II**

### Paper- IV

### **Spectroscopy & Computer for Chemist**

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
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Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT)	internal
	<b>MM 80</b>

### Unit-I

**Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin Nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant \_JI, Classification (ABX, AMX, ABC, A<sub>2</sub>B<sub>2</sub>,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 FTNMR,advantages of FT - NMR use of NMR in medical diagnostics.

### Unit-II

**X-Ray Diffraction:** Bragg condition Miller indices, Laue Method, Bragg Method, Debye-Scherer method of X-ray structural analysis of crystals, index reflections, identifications 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.

**Electron Diffraction:** Scattering intensity Vs scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecule. Low energy electron deffraction and structure of surfaces.

**Neutron Diffraction:** Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

### Unit-III

**Electron Spin Resonance Spectroscopy:** Basic principles zero field splitting and Kramers degeneracy, factors the —gl value isotopic and anisotropic hyperfine coupling constant, spin Hamiltonian, spin densities and McConnell relationships, measurement techniques, applications.

**Nuclear Quadrupole Resonance Spectroscopy:** Quadrupole nuclei, Quadrupole moments, electronic field gradient, coupling constant, splitting, Applications.

### Unit-IV

**Introduction to computers and computing:** Basic structure and functioning of computers with a PC as an illustrative examples. Memory, I/O devices, secondary storage, computer languages, oprating systems with DOS as an example. Introduction to UNIX & WINDOWS. Data processing, principles of programming Alogorithms and flow charts.

**Computer Programming in FORTRAN/ C / BASIC:** The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the feature may be replace appropriately). Elements of computer language, Constant and Variables. Operations and Symbol. Expressions. Arithmetic assignment statement. Input and Output. Format statement, Termination statements. Braching statements such as IF or GO TO statement LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement

### **Books Suggested:-**

1. Modern Spectroscopy J. M. Hollas, John Willey.

2. Spectroscopy, H. Kaur, Pragati, Prakashan

3. Molecular Spectroscopy, Banwall.

4. Molecular Spectroscopy, P. S. Sindhu, New Age International.

5.NMR, NQR, EPR, and Mossbauer Spectroscopy in Inorganic Chemistry, R. B. Perish, Ellis Horwood.

6.An Introduction to Spectroscopy, S. S. Kalra, Anusandhan Prakashan

7.Computer for Chemists; K.V. Raman.

8. Computer Programming in FORTRAN IV and V, Rajaraman, Prentice Hall.

9. Computational Chemistry, A. C. Norris.

10.Computer for Chemists, Singh and Mishra, Anusandhan Prakashan.

11. Fundamentals Spectroscopy, S.P.S. Jadon, Anusandhan Prakashan

## SEMESTER-II LABORATORY COURSE - 03 Organic Chemistry

### **MM 100**

## General Methods for Separation and Purification of Organic Compounds with Special reference to:

1. Solvent Extraction

2. Fractional Crystallizations

### **Distillation Techniques:**

Simple distillation, Steam distillation, Fractional distillation and Distillation under reduced pressure.

### **Analysis of Organic Binary Mixture:**

Separation and identification of organic binary mixtures containing

two components

### (A student is expected to analyze at least 10 different binary mixtures.)

### **Preparation of Organic Compounds: Single Step Preparation:**

- Acetylation: synthesis of β Naphthyl acetate from β-Naphthol / Diacetate from Hydroquinone.
- Aldol condensation: Dibenzal acetone from benzaldehyde.
- Bromination: p-bromoacetanilide from acetanilide.
- Canizzaro reaction: Benzoic acid and benzyl alcohol from benzaldehyde.
- Friedel crafts reaction: O-benzoyl benzoic acid from phthalic anhydride.
- Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.
- Oxidation: Adipic acid by chromic acid oxidation of cyclo-hexanol.
- Perkin's reaction: Cinnamic acid from benzaldehyde.
- Sandmeyer reaction: p-chlorotoluene from p-toluidine/O-chlorobenzoic acid from anthranilic acid.
- Schotten Baumann Reaction: β-Naphthyl benzoate from: β-Naphthol / phenyl benzoate from phenol.
- Sulphonation reaction: Sulphanilic acid from aniline.
- Nitration: p-nitroacetanilide from acetanilide.
- Hydrolysis: p-nitroaniline from p-nitroacetanilide and bromoaniline from pbromoacetanilide.

## **Books Suggested:**

1. Practical Organic Chemistry by A. l. Vogel.

2. Practical Organic Chemistry by Mann and Saunders.

3. Practical Organic Chemistry by Garg and Saluja.

4. The Systematic Identification of Organic Compounds by R.L. Shriner and D.Y. Curtin.

5.Semi micro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and J.B. Entrikin and

E.M. Hodnett.

6.A Handbook of Organic Analysis by H.T.Clarke.

7. Advanced Practical Organic Chemistry by O.P. Agrawal

### SEMESTER -II

### **LABORATORY COURSE - 04**

### **Analytical Chemistry & Computers**

### **MM 100**

### Part-A. Analytical Chemistry

### Error Analysis and statistical data analysis.

Errors, types of errors, minimization of errors, statistical treatment for error analysis, standard deviation, method of least squares. Calibration of volumetric apparatus, burettes, pipettes, standard flask, weight box etc.

### **Volumetric Analysis**

Determination of iodine and saponofication values of oil samples, Determination of DO, COD, BOD, hardness of water sample.

### Solubility:

Determination of solubility of an inorganic salt in water at different temperature and hence plot the solubility curve.

Determination of transition temperature by solubility method.

### Chromatography

Separation of inorganic ions and amino acids by paper chromatography,

column chromatography.

Separation and identification of the sugars present in given mixture of glucose, fructose and sucrose bypaper chromatography and determination of  $R_f$  values.

Thin - layer chromatography:

Separation of Ni, Mn, Co, and Zn and determination of Rf values.

### **Conductance of Electrolyte:**

Determination of basicity of organic acids.

Determination of degree of hydrolysis and hydrolysis constant of CH<sub>3</sub>COONa & NH<sub>4</sub>Cl

### Flame Photometry/AAS/FIA

Determination of cations, anions and metal ions e.g. Na, K, Ca, SO<sub>4</sub>, NO<sub>2</sub>, Fe, Mo, Ni,

### Spectrophotometry

Verification of Beer's law. Molar absorptivity calculations, plotting graph to obtain max etc.,

Study of colour change and pH range of some indicators.

Determination of some metal ions in various environmental samples.

## **Nephlemetry / Turbidimetry**

Determination of chloride, sulphate, phosphate, turbidity etc.

### **Part-B** Computer

Use of computer programmers: The students will learn to operate a PC and hope to run standards programmers and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmers. Monte Carlo and molecular dynamics, programmers with data preferably from physical chemistry laboratory. Further the students will operator one or two packages such ads MATLAB, EASYPLOT, LOTUS, FOXPRO and word processing software such as WORDSTAR / MS- WORD.

Development of small computer course involving simple formulae in chemistry, such as Vanderwalls equation. PH titration, kinetics, radioactive decay. Evolution of lattice energy and ionic radio from experimental data linear simultaneous equation to solve secular equations within the Huckel theory. Elementary structural feature such as lengths, bond, dihedral angles etc. of molecules extract base such as Cambridge database.

## **SEMESTER-IV**

## **DISTRIBUTION OF MARKS**

## **THEORY (16 CREDITS)**

			Marks		
No.	Name of Paper				Credit
		Theory	Internal assessment ( Unit Test)	Total Marks	Points
Ι	Photo-inorganic & Bioinorganic Chemistry	80	20	100	04
Π	Medicinal Chemistry	80	20	100	04
III	Physical Organic & Nuclear Chemistry	80	20	100	04
IV	Spectroscopy	80	20	100	04

## PRACTICAL (4 CREDIT)

Course	Paper	Marks	Two Experiment	Viva	Sessional	Credit	Time
Practical-1	Inorganic Chemistry	100	60	20	20	02	10 Hr
Practical-2	Physical Chemistry	100	60	20	20	02	8 Hr

### **SEMESTER-IV**

### Paper I Photo-inorganic & Bio-inorganic Chemistry

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT) .	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
I Init-I	IVIIVI 80

Metal Storage Transport and Bio mineralization: - Ferritin, transferrin and siderophores.

Na+/K+ Pump: - Role of metal ions in biological processes.

**Calcium in Biology:** - Calcium in living cells, transport and regulation, molecular aspects of intermolecular processes, extra cellular binding proteins.

**Metals in Medicine:** - Metal deficiency and disease, toxic effects of metals for diagnosis and chemotherapy with particular reference to anti cancer drugs.

### Unit- II

**Biogenetics and ATP Cycle:** - DNA polymerization, glucose storage metal complexes in transmission of energy, chlorophylls, photosystem-I and photosystem-II cleavage of water molecule system.

**Electron Transfer in Biology: -** Structure and function of metalloproteins in electron transport processes-cytochromes and iron sulphur proteins, synthetic models.

**Transport and storage of Dioxygen:** - Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, haemocyanins and haemerythrin, model synthesis complexes if iron cobalt and copper.

**Metalloenzymes:** Metalloenzymes: - Zinc enzymes-carboxypeptidases and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzymes-Super oxide dismutase ,Molybdenum oxatranferase enzymes-xanthine oxidase.

### Unit- III

**Basics of Photochemistry:** - Absorption, excitation, photochemical laws, quantum yield, electrically excited states-life times-measurement of the times, flash photolysis, Absorption spectra, frank-Condon principle, photochemical stages-primary and secondary processes, structure dipole moment, acid base strength, reactivity of excited state.

### Unit- IV

**Photochemical Reactions:-** Photo oxidation-reduction reaction, photo isomerisation reaction, Photochemistry of carbonyl complexes and mixed ligand carbonyls. Photo dissociation reaction, photo exchange reaction, photo substitution reaction, photosensitized leads to polymerization and miscellaneous reactions..

**Photochemistry of mixed ligand complexes containing bonding organic ligands**:-Photochemistry of chromium, manganese and iron complexes. Photoexchange, photoaquation, photoanation reactions, Admsons rule, photolysis mechanism, energy convertion and photochemical decomposition of water.

### **Book Suggested: -**

1.Bioinorganic Chemistry. I. Bertini, H.B. Gray, S. L. Lippard and J. S. Valentine, University Science Books.

2. Inorganic Biochemistry Vols-II and I. Ed G.L. Eichhorn, Elsevier.

3. Enzyme Chemistry Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.

4. Enzyme Mechanisms, M.I. Page and A. Williams, Royal Society of Chemistry.

5. Fundamentals of Enzymology, N.C. Price and L. Stevens Oxford University Press.

6.Enzyme Structure and Mechanisms, A. Fersht, W. H. Freeman.

7. Macromolecules: structure and Function, F. Wold. Prentice hall.

8. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.

9. Inorganic Photochemistry, J. Chem. Educ, Vol.60, no. 10, 1983.

10. Progress in inorganic Chemistry, Vol. 30, ed. S.J. Lippard, Wiley.

11.Coordination Compounds, V. Balxari and V. Carassiti, Academic press.

12.Coordination Chem.Revs, 1981, Vol.39, 121, 131, 1975, 15, 321, 1990, 97, 313.

13. Elements of Inorganic Photochemistry, G.J. Ferraudi, Wiley.

## SEMESTER –IV Paper-II Medicinal Chemistry

### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) from all FOUR unit. Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) with internal choices (06 marks for each UNIT).

Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) internal with choice (12 marks for each UNIT).

## **MM 80**

### Unit-I

**Drug Design:** - Development of new drugs, procedure followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, Structure activity relationship (SAR), factors affecting bioactivity, Quantitative structure activity relationship (QSAR), Concept of drug receptors, Physico-chemical parameter, lipophylicity, partition coefficient, Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson and Hansch analysis, LD-50, ED-50 (Mathematical derivation of equations. excluded).

### Unit-II

**Pharmacokinetics:** - Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics', Methods and uses of pharmacokinetics in drug development process.

**Pharmacodynamics:** - Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

### Unit-III

**Local Anti Infective Drugs:** - Introduction and general mode of action, Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole and griseofulvin.

**Antimalarials:** - Synthesis and properties of the following anti malarial, 8-amino quinoline derivatives-pamaquine, primaquine, pentaquine, isopentaquine, 4-amino quinoline, derivatives-santoquine, camaquine, acridine derivatives-mepacrine, azacrin, pyrimidine and biquanide, derivatives-paludrine, pyremethamine.

**Antibiotics:** - Cell wall biosynthesis, inhibitors,  $\beta$ -lactum rings, antibiotics, inhibiting protein synthesis, synthesis of Penicillin-G, Penicillin-V, Ampicillin, Amoxycillin, Chloramphenicol, Cephalosporin, Tetracyclin and Streptomycin.

### Unit-IV

**Cardiovascular Drugs:** - Introduction, Heart anatomy and Cardiac cycle, Electro Cardio Gram (E.C.G.), cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amylnitrate, qunidine methyldopa, sorbitrate and atenolol, Varapamil.

**Antineoplastic Drugs:** - Introduction, cancer chemotherapy, special problems, role of alkylating agents and anti metabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards and 6-mercaptopurine.

### **Book Suggested: -**

1. Natural Products Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs.

2.Organic Chemistry, D.V. Banthrope, Longman Essex, J. B. Harbrone.

3.Streoselective Synthesis, M.Nogradi and CHV. Odds Chemistry of Carbon Compounds, ED.S. Coffey, Elsevier.

4.Biological and Pharmacological Properties of Medicinal Plants from Americans, M. 5.P. Gupta and A. Marston, Harwood Academic Publishers.

6.Introduction to Flavonoids, B. A. Bohm. Harwood Academic Publishers.

7.New Trends in Natural Products, Rahman and M.I. Choudhary.

8.Insecticides of Natural Origin, Sukh Dev.

9. Text Book of Organic Medicinal and Pharmaceutical Chemistry, Robert F. Dorde.

10.An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock.

11.Berger's Medicinal Chemistry and Drug Discovery, Vol-I (Chapter-9 and Ch-14).

12.Goodman and Gillman's Pharmacological Basis of Therapeutics, Mc Graw Hill.

13. The Organic Chemistry of Drug Design and drug Action, R.B. Silverman.

14. Strategies for Organic Synthesis and Design, D. Lednicer, John Wiley.

### SEMESTER IV

### Paper-III

### **Physical-Organic and Nuclear Chemistry**

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT) .	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
	<b>MM 80</b>

### Unit-I

**Kinetic Isotope Effect:** - Theory of isotope effects; Primary and secondary kinetic isotope effects; Heavy atom isotope effects; Tunneling effects; Solvent effects.

**Structural Effect on Reactivity:** - Linear free energy relationships (LFER) .The Hammett equation, Substituent constants; Interpretation of  $\sigma$  –values. Reaction constant p. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant The Taft model and  $\sigma_1$ - and  $\sigma_R$  -scales.

**Solvent Effects:** - Introduction, the concept of solvent polarity. Qualitative theory of the influence of the solvent on reaction rate. The treatment of solvent effects on reaction rate in term of dielectric constant. Solvent parameters. Detailed analyses of solvent effects.

### Unit-II

**Steric and Conformational Properties:** - Various types 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. Winstein- Holness and Curtin- Hammett principle.

Acid Base, Electrophiles, Nucleophiles and Catalysis: - Acid-base dissociation, Electronic and structural effect ;acidity and basicity; Acidity functions and their applications Nucleophilicity scales, Nucleofugacity. The  $\alpha$ - effect, acid- base catalysis-specific and general catalysis. Bronsted catalysis, nucleophilic and electrophilic catalysis. Catalysis by non- covalent binding Micellar catalysis.

### Unit-III

**Nuclear Theory:** - Nuclear cross section and nuclear radii, nuclear shells and magic numbers, theory of nuclear shell model, nuclear potentials, square well potential and simple harmonic oscillator potential, liquids drop model. Semi-empirical mass equation, application and limitation.

**Radioactivity:** - Radioactivity decay and equilibrium decay kinetics, modes of radioactive decay, alpha decay, and beta decay.

**Detection of Nuclear Radiations:** - Techniques, equipments, G.M. counter, proportional counter, Scintillation counter, counting statistics.

### Unit-IV

**Nuclear Reactions:** Q-values, energetic, cross sections, resonance, compound nucleus theory of nuclear reaction, types of nuclear reactions chemical effects of nuclear transformations, Szilard-Chalmer Reaction and recoil chemistry, retention.

**Nuclear Fission:** - Mass, energy and charge distribution of fission products, decay chains and delayed neutrons, liquid drop model of nuclear fission.

**Nuclear energy:** - Nuclear fission, chain reaction multiplication factor, homogenous and heterogeneous reactor, and reactors.

### **Book Suggested:**

1.Introduction to Theoretical Organic Chemistry and Molecular, Modeling W.B. Smith, VCH Weinheim.

2. Physical Organic Chemistry, N. S. Isacs, ELBS/Longman.

3.Correlation analysis in Organic chemistry, John Shorter, Oxford Chemistry Series.

4. Advanced in linear free energy relationship, N. B. Chapman and J. Shorter, Plenum press.

5.Correlation analysis of Organic chemistry, John Shorter, Research studies press (A division of J. Wiley & Sons Ltd.).

6. The Hammett equation, C. D. Johnson, Cambridge University press.

7.Nuclear Radiochemistry by G. Friedlander, J.W. Kennedy & J.M. Miller, John Witter & Sons, Ine New York.

8. Source Book Atomic Energy, S. Gladstone, Affiliated East-West Press Pvt. Ltd. New Delhi.

9. Nuclear Physics by I. Kaplan, Addison, Wesley, Publishing Company.

10.Nuclear Chemistry and its Applications. M. Haissinky, Adision Wesley, Publishing Company, London.

11.Essential of Nuclear Chemistry, H.J. Arnikar, Wiley Eastern Ltd New Delhi

### SEMESTER –IV

### Paper-IV

### Spectroscopy

#### QUESTION PAPER WILL BE DIVIDED INTO THREE SECTIONS.

Section –A [Multiple choice/Objective Type]. This section contains EIGHT questions (1 marks each) FOUR unit.	from all
Section –B [Short answer type]. This section contains TWO questions from each unit (Total 08 Que) internal choices (06 marks for each UNIT).	with
Section –C [Long answer type]. This contains ONE question from each unit (Total 04 Que) with choice (12 marks for each UNIT).	internal
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### Unit-I

**Nuclear Magnetic Resonance Spectroscopy**: -The Contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications. chemical shift, spin-spin, interaction. Shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefin, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides 7 mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (First order spectra), Virtual coupling spectrochemistry, hindered rotation, karplus curve-variation magnetic double resonance, contact shift reagents, solvent effect,

### Unit-II

**Carbon- 13 NMR Spectroscopy**: - General consideration, chemical shift (aliphatic, olefinic, alkynes, aromatic, heteroaromatic and carbonyl carbon), coupling constant. Two imension NMR spectroscopy-COSY, NOES, DEPT, APT and Inadequate techniques.

**Photoacoustic Spectroscopy:** Basic principles of photoacoustic spectroscopy (PAS), PAS-gasses and condensed system chemical and surface applications.

### Unit-III

**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 PH4, F<sub>2</sub>- and [BH<sub>3</sub>]-**Vibrational Spectroscopy:** -

Symmetry and shapes of AB2, AB3, AB4, AB5 and AB6 mode of bonding of ambidentate legends, ethylendediamine and diketonato complexes, application of resonance spectroscopy particularly for the study of active sites of metalloproteins.

## Unit-IV

## Mass spectroscopy:

Basic principle, fragmentations, Base peaks, Mclafferty rearrangement, applications,

## Mossbauer Spectroscopy:

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

## Book Suggested: -

1. Physical Method of 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 Raman Spectra, Inorganic and Coordination Compounds, K. Nakamoto, Wiley.

4. Progress in Inorganic Chemistry Vol. 8ed, F.A. Cotton Vol. 15. ed. S.J. Lippard, Wiley.

5. Transition metal Chemistry, R. L. Carlin Vol.3, and Dekker.

6.Inorganic Electronic Spectroscopy, A.P.B. Elsevier.

7.NMR, NQR, EPR and Mossbauer Spectroscopy in inorganic Chemistry, R.V. Parish, Ellis Harwood.

8. Practical NMR Spectroscopy, M.L.Martin, J.J. Delpeuch and G.L. Martin, Hyen.

9.Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morril, John Wiley.

### SEMESTER – IV

### **LABORATORY COURSE - 03**

### **Inorganic Chemistry**

## Time- 10 Hrs

### A. Quantitative Analysis:

Quantitative separation and determination of three-component system using standard volumetric and gravimetric methods of analysis. The system can be any one of the following.

- (I) Cu, Ag & Zn
- (II) Cu, Ni & Zn
- (III) Fe, Al & Ca
- (V) Ag, Ni & Zn
- (VI)Ba,Ni,Zn

### **B.** Analysis of alloys ores and minerals.

- (I) Ni alloy
- (II) Cu, Ni, Zn alloy
- (III) Steel
- (IV) Lime stone and dolomite: Silica, Sesqui oxide (R<sub>3</sub>O<sub>3</sub>), Ca, Mg, L.O.I.etc.
- (V) Haematite: Iron, Al, Ca, Mg. Acid insoluble & silica etc.
- (VI) Bauxite: Silica, Fe, Al, Be, Ti etc.
- (VII) Cement: Silica, Fe, Al, Ca, and Mg & SO-24 etc.

C. Inorganic Reaction Mechanism: Kinetic and mechanism of following reaction:

(I) Substitution reaction in octahedral complexes (acid hydrolysis and base hydrolysis.

- (II) Redox reaction in octahedral complexes.
- (III) Isomerisations reaction of

### octahedral. D. Preparation:

- Preparation of selected Inorganic complexes and other inorganic compounds and their study by IR, electronic, Mossbauer and ESR, spectra and magnetic susceptibility measurements.
- Synthesis & thermal analysis of group II metal oxalate hydrate.
- Preparation of Tin (IV) & Iodide, Tin (IV).
- Chloride and Tin (II) Iodide. .
- Synthesis of metal acetylacetonate; Magnetic moment, IP, & NMR,
- Bromination of Cr(acac)<sub>3</sub>

### MM 100

- Cis and Trans  $[Co(en)_2Cl_2]^+$ .
- Separation of optical isomer of cis [Co(en)<sub>2</sub>Cl<sub>2</sub>]NO<sub>3</sub>.3H<sub>2</sub>O, [Cr(H<sub>2</sub>O)<sub>4</sub>Cl<sub>2</sub>]Cl.2H<sub>2</sub>O and [Cr(en)Cl<sub>3</sub>]. [Cr(acac)<sub>3</sub>],
- Reaction of Cr (III) with a multidentare ligand; a kinetic experiment (visible spectra Cr.-EDTA complex).
- Preparation of [Co (phenonthroline –5, 6-quinone].
- Preparation and use of Ferrocene.
- Prep of copper glycine complex cis and trans- bis [glycinato Copper (II)]
- Preparation of phosphine PH3P and its transition metal complexes.
- Any other experiment such as conversion of p-xylene to terphthalic acid catalyzed by CoBr<sub>2</sub>(homogeneous catalysis).
- Extraction of chlorophyll from green leaves of students of choice. Separation of chlorophylls and their electronics spectral study.
- Complexation study of Cu (II) ion with biologically important amino acids.

## **Books Suggested:**

1.A.W. Adamson and P.D. Fleischaner: Concept of Inorganic Photochemistry.

2.V. Balzani and V. Carassiti: Photochemistry of coordination compounds.

3.K. K. Rohatgi and Mukherjee: Fundamentals of Photochemistry.

- 4. Quarterly Reviews; 21, 213, (1967).
- 5. Coordination Chemistry Reviews 3, 169, (1968).
- 6.Quarterly Reviews; 8, 422 (1954).
- 7.G. L. Eichhorn: Inorganic Biochemistry Vols I.II.

8.M.W. Hughes: Inorganic Chemistry of Biological Process.

8. Purcell and Kotz: inorganic Chemistry.

9.R.C. Mehrotra and A. Singh: Organometallic Chemistry An Introduction.

10. J. J. Lagowski: Modern Inorganic Chemistry.

11.Cotton and Wilkinson 5<sup>th</sup> Edition Advance Inorganic Chemistry.

## SEMESTER – IV Physical Chemistry Practical

## Time- 10 Hrs

## A.Conductometry

To verify Debye Huckel and Onsagers limiting law for strong electrolyte. Determination of the solubility, solubility product of sparingly soluble salt(Lead iodide,Barium sulphate etc.)

To determine the degree of hydrolysis constant of (i) CH<sub>3</sub> C00Na and (ii)

## NH<sub>4</sub>Cl **B.Colorimetry**

To determine the indicator constant pka of methyl red spectrophotometrically.

To verify additivities of absorbance of a mixture of a colored substance in a solution using

KMnO4 / K2Cr2O7 solutions.

To determine the dissociation constant phenolphthalein colometerically.

## C.pH Metry

To determine pKa of given dibasic and tribasic acid.

To determine the pH of various mixtures of acetic acid & Sod. -acetate in aqueous solution and determine the dissociation constant of the acid.

## **D** Potentiometry

Titrate ferrous ammonium sulphate against  $K_2Cr_2O_7$  /KMnO<sub>4</sub> and determine redox potential of

ferrous/ferric system.

To determine ionization constant of polybasic acid.

Determination of the dissociation constant of Barium Nitrate.

Titrate a weak acid( e.g. acetic acid, benzoic acid. Oxalic acid etc.)

potentimetrically and determine the dissociation constant of the acid.

## E. Distribution Method, Partial Molar Volume

To determine the formula of the complex formed between cupric ion & ammonia by distribution method.

Determine the equilibrium constant of the following reaction  $KI+I_2 = KI_3$ 

Determine the partial molar volume of NaCl in aqueous Solutions at room temperature.

Determination of the partition coefficient for iodine between carbon tetrachloride/kerosene oil & Water

## MM 100

## F. Chemical Kinetics

To study the effect of temperature concentration of the reactant is a catalyst on the rate of
To study the effect of temperature, concentration of the reactant is a catalyst on the
a chemical reaction.
Saponification of ethyl acetate (a) Volumetric method (b) Conductometric method.
Reaction between acetone and iodineTo study the autocatalytic reaction between KMnO <sub>4</sub> and
Oxal c acid.
Reaction between $K_2S_2O_8$ and $I_2$
Study the kinetics of decomposition of the complex formed between Sodium sulphide and
Sod. Nitropruside spectrometrically.
Determine colorimetrically the order and the energy of activation for decomposition of
violet coloured complexs of ceric ions and N- phenyl anthranilic acid.
Reference Books :-
1.Advance Practical Physical Chemistry- Dr. J.B. Yadav Krishna Prakashan Media(P) LTd, Meerut.
2.Senior Practical Physical Chemistry Dr. B.D. Khosla, V.C. Garg, Adarsh Gulani- R. Chand & W
New Delhi.
3. Experiments in Physical Chemistry by Dr. J.C. Ghosh- Bharati Bhawan.
4. Advanced Practical Chemistry R. Mukhopadhyay, P. Chatterjee- Books and allied(P) Ltd Kolkatta.

5. Chemical analysis and instrumental approach by A.K. Shrivastava & P.C. Ltd, New Delhi.