

M.G.S. UNIVERSITY, BIKANER SYLLABUS

FACULTY OF SCIENCE

M.Sc. CHEMISTRY
M.Sc. Previous Examination - 2020
M.Sc. Final Examination - 2021



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Maharaja Ganga Singh University, Bikaner

- (i) Thermal analysis - Thermal composition of calcium oxalate, copper sulphate, calcium sulphate, hydrate.
- (ii) Electro Gravimetric analysis- Separation & determination of nickel & carbonate.
- (iii) Atomic absorption spectroscopy- Determination of zinc & copper
- (vi) Flame photometry- Determination of Sodium, calcium, magnesium & potassium.
- (v) IR Spectro photometry- Sample preparation, Identification of functional groups.
- (vi) Experiments related with computational and virtual chemistry may be designed and performed.

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes and a separate copy shall be used for the purpose

Instructions to Examiners

Five exercises are to be given in examination, selecting not more than one exercise from A to H.

Marking Scheme

Exercise	Marks
Exercise No. 1	20
Exercise No. 2	20
Exercise No. 3	20
Exercise No. 4	20
Exercise No. 5	20
Spotting	10
Viva	10
Record	10
Seminar & Project Works	20
Total	150

Note: Seminar Marks will be awarded by panel of examiners / experts (which will conduct seminars) constituted internally by Head of the department which will be hand over it to the board of examiners. It is advised to conduct two seminars one in the mid of the session and one at the end of the session

SYLLABUS & SCHEME OF EXAMINATION FOR M.Sc. CHEMISTRY (Two Year Course)	
M.Sc. (Previous) Chemistry, 2020	
Papers	Max. Marks
(i) Determination of very weak acid eg. Vaniline, Isovaline, phenolic compounds etc.) using base (e.g. Lithium hydroxide, barium hydroxide etc.)	75
(ii) Study of Precipitation and/Complex formation reaction by drawing titration curve eg. silver salt with lithium chloride, ammonium sulphate with barium acetate, etc.	75
(iii) Determination of cations Iron (II) as or anions eg- chloride, dihydrogen phosphate	75
(iv) Determination of free acid in solution of metal salt (e.g. sulphuric acid/ in aluminium sulphate, Perchloric acid in uranyl pechlorate)	75
(B) Potentiometric/pH Metric method:-	Total Marks 450
(i) Determinations of metal-ions, eg. Iron (ii), Copper (ii), Chromate (ii), Manganese (ii) in pyrolusite/steel etc.	M.Sc. (Final) Chemistry, 2021
(ii) Determination of metal-ion eg. Calcium (II), Nickel (II) Cobalt (II), Zinc (II) etc	75
(C) Polarographic Method:-	75
(i) Determination of half wave potential & metal ions eg. Cadmium (II), Mercury (II), Copper (II) etc.	75
(ii) Determination of metal-ions, eg. Cadmium (II), Mercury (II), Copper (II) etc, using wave height concentration cell or standard addition.	75
(iii) Investigation of the influence of dissolved oxygen.	75
(iv) Determination of lead and copper in steel.	75
(D) Amperometric Method	Group-A
(i) Determination of lead with std. potassium dichromate solution	VII(a) Advanced Inorganic Chemistry 75
(ii) Determination Nickel (ii) with dimethyl glyoxime.	VII(b) Metal Complexes, Polymers and ceramics 75
(iii) Determination of Zinc with EDTA	Group-B
(iv) Determination of water content of salt hydrate	VIII(a) Organic Synthesis 75
(E) Chromatographic Separation	VIII(b) Heterocyclics and Natural Products 75
(i) Separation of Zinc(II) & Magnesium (II) on an Ion exchanger.	Group-C
(ii) Separation of chloride & bromide on an Ion exchanger.	IX(a) Recent Trends in Physical Chemistry 75
(iii) Separation & recovery of dyes (eg. bromophenol blue, Congo red, phenol red) using TLC.	IX(b) Computational Chemistry 75
(iv) Separation of artificial colorant in confectionery by TLC	Group-D
(F) Solvent Extraction:	X(a) Analytical chemistry 75
(i) Separation & determination of Copper (II) as diethyldithio carbamate complex.	X(b) Applied Analytical Chemistry 75
(ii) Separation & Determination of Copper (II) as Neocuproin complex.	Practical
(iii) Separation & determination of Iron (II) as 8-hydroxy quinolate.	(Including 20 marks for Project work and Seminar) 150
(G) Spectrophometric Determination.	Total Marks 450
(i) Determination of Boron/Chromium/Titanium/tungsten in steel.	Grand Total 900
(ii) Simultaneous determination - Chromium (II) & Manganese (II).	Note :-
(iii) Determination of active constituents in a medicine by derivative spectroscopy e.g. two drugs pseudoephedrine hydrochloride and tcioprolidine hydrochloride in "Actified" a medical preparation.	1 Papers with 75 marks will be taught for four hours/week.
(iv) Determination of cholesterol.	2 Practical (both M.Sc. Previous & Final will cover 24 hours/ week).
(H) Other methods -	3 Project work and seminars (case study report with presentation) will be assigned one hour/week for M.Sc. Final Year.
	4 Panel of Examiners - A panel of Three examiners will conduct Practical examination (for each batch of M.Sc. Previous and Final) among which at least One will be External Examiner.
	5 Marking scheme & pattern of each Theory paper is given as
	1 Each Theory paper will be of 75 marks (Minimum passing marks-19 each paper). There will be Four theory papers and total marks in

- Theory papers will be 300 (Aggregate minimum passing marks-108).
 Time duration for each paper will be 3 hours
- The Practical exam will be of 150 marks (minimum passing marks 54). Practical exam will be of 14 hours spread over 2 days.
 - Each Theory paper will be divided into three Sections i.e. A, B and C.
 - Section A will contain 10 questions (two questions from each unit), all questions are compulsory carrying 2 marks (Answer limit 50 words)
 - Section B will contain 10 questions (two questions from each unit), Student will have to answer total 5 questions (attempting 1 question from each unit) carrying 5 marks (Answer limit 200 words).
 - Section C will contain 5 questions (one question from each unit). Student will have to answer total 3 questions as per their choice, out of these 5, carrying 10 marks each question (Answer limit 500 words)

Marking Scheme	Exercise	Marks
	Exercise No. 1 (from Section A)	30
	Exercise No. 2 (from Section B)	25
	Exercise No. 3 (from Section C)	25
	Exercise No. 4 (from Section D)	15
	Exercise No. 5 (from Section E or F)	15
	Viva	10
	Record	10
	Seminar & Project Work	20
	Total	150

M.Sc. (PREVIOUS) CHEMISTRY, 2020.

PAPER-I CH-401 INORGANIC CHEMISTRY

Time : 3 Hours

Max. Marks :75

UNIT-I

(a) Stereochemistry and Bonding in main group compounds : VSEPR, Walsh diagrams (Tri and penta- atomic molecules), dp-pp bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

(b) Metal-Ligand Equilibria in Solution : Stepwise and overall formation constants and their interaction, trends in stepwise constant, 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.

Unit-II

Reaction Mechanism of Transition Metal Complexes: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, 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 reactions. 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.

Unit-III

(a) Metal - Ligand Bonding : Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, bonding and molecular orbital theory.

- Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
- Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan.
- Green Chemistry : An experimental study, R.K. Sharma, N. Bhojak, I.T. Sidhwani and M.K. Choudhary

Instructions to Examiners
 Five exercises are to be given, selecting one exercise from section A to D and fifth exercise is to be selected from section E or F.

Note: Seminar Marks (for Project Work & Seminar) will be awarded by panel of examiners/ experts (which will conduct seminars) constituted internally by Head of the department which will be hand over it to the board of examiners. It is advised to conduct two seminars one in the mid of the session and one at the end of the session.

Books Suggested:

- Inorganic Experiments, J. Derek Woollins, VCH.
- Microscale Inorganic Chemistry, Z. Szafran, R.M Pike and M.M. Singh, Wiley.
- Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
- The Systematic Identification of Organic Compounds, R.L Shriner and D.Y. Cuten.
- Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett.
- Experimental Organic Chemistry, M.P. Doyle and W.S. Mungall.
- Small Scale Organic Preparations, P.J. Hill.
- Organometallic Synthesis, J.J. Fisch and R.B. King, Academic.
- Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGrawHill Interscience.
- Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
- Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan.

M. Sc. (FINAL) CHEMISTRY PRACTICAL ANALYTICAL CHEMISTRY

Time: 14 Hours (Spread in 2 Days) (Including 20 Marks for Project Work & Seminar)

(A) Analysis & Determinations (Marks 25 each)

- (b) To plot the characteristics of a transistor used as a diode and compare the results with those of (a)
2. To implement a diode clipper circuit for the given transfer characteristics and verify the wave form.
3. To implement a diode clamper circuit which clamps the positive peak of the input voltage to (a) Zero voltage and (b) a given voltage. Verify the performance.
4. (a) To Plot the characteristics of an NPN transistor in CE configuration, (b) To find the h-parameter of the transistor from the characteristics.
5. (a) To plot the characteristics of an NPN transistor in CB configuration. (b) To find the h-parameter of the transistor from the characteristics and compare it with the results of experiment No. 6
6. (a) To plot the drain and transfer characteristics of JFET in CS configuration, (b) To find out the pinch off voltage, maximum drain to source saturation current and the trans conductance.
7. To obtain the frequency response of an RC coupled amplifier and estimate the bandwidth.
8. (a) To Plot the characteristics of Zener diode and find its dynamic resistance under reverse biased condition (b) To use zener diode for a. voltage regulation (i) Plot the line regulation curve, (ii) Plot the low regulation curve.
9. (a) To wire a half wave Rectifier circuit using diode and measure the rms voltage, dc voltage and to find Ripple factor. (b) To study the performance of Half wave and full wave doubler circuits.
10. To plot characteristics of UJT and find the peak voltage, peak current and valley voltage and use as a relaxation.
- Note: A Sheet containing 20 questions/diagrams/circuits will be provided to the students to reply. These questions based on basic electronics will cover both theory and practicals as provided in the syllabi. They will be of objective type for duration of 20 minutes with maximum scoring of 10 marks.
- Books Suggested:**
- Inorganic Experiments, J. Derek Woollins, VCH.
 - Microscale Inorganic Chemistry, Z. Szafran, R.M Pike and M.M. Singh, Wiley.
 - Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
 - The Systematic Identification of Organic Compounds, R.L Shriner and D.Y. Cutin.
 - Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett.
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 - Small Scale Organic Preparations, P.J. Hill.
 - Organometallic Synthesis, J.J. Fisch and R.B. King, Academic.
 - Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGrawHill Interscience.
- (b) Metal Clusters :** Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.
- (c) Symmetry and Group theory in chemistry-** symmetry elements and symmetry operation, definition of group sub group, relation between orders of a finite group and subgroup conjugacy relation and classes. Point symmetry group Schoenflies symbols representation of groups by matrices. Character of a representation. The great orthogonality theorem and its importance Character tables and their use.
- Unit-IV**
Electronic spectra and magnetic properties of transition metal complexes spectroscopic ground states, correlation, Orgel and Tanabe-sugano diagram 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 chemical information, magnetic moments magnetic exchange coupling and spin crossover.
- Unit-V**
(a) Metal p Complexes : Metal carbonyls, structure and bonding, vibration spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, structure and important reactions of transition metal nitrosyl, dinitrogen and deoxygenate complexes; tertiary phosphine as ligand.
(b) Green chemistry Principles and applications in synthesis and analysis. Safety rules and safe use of different materials and chemical and biochemical weapons.
- Books Suggested :**
- Advanced inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
 - Inorganic Chemistry, J.E. Huhey, Harpers & Row.
 - Chemistry of the elements, N.N. Greenwood and A. Earnsho, Pergamon.
 - Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
 - Magneto chemistry, R.L. Carlin, Springer Verlag.
 - Comprehensive Coordination Chemistry eds. G. Wilkineson, R.D. Gillars and J.A. McCleverty, Pergamon.
 - Green Chemistry Theory and Practice, Paul T. Anastas and John C. Warner, Oxford University Press.
- PAPER-II CH-402 ORGANIC CHEMISTRY**
Time : 3 Hours **Max Marks :75**
- Unit-I**
(a) Nature of Bonding in organic Molecules : Delocalized chemical bonding—conjugation, cross conjugation, resonance, hyperconjugation, bonding influence tautomerism.
Aromaticity in benzenoid and non-benzenoid compounds alternant and non alternant hydrocarbons, Huckel's rule, energy level of molecular orbital, annulenes, anti aromaticity, Psi aromaticity homo aromaticity. PMO

approach. Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds cyclodextrins, catenane and rotaxanes.

(b) Stereochemistry : Conformational analysis of cycloalkanes, decaline, 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 method of resolution, optical purity enantiotropic and diastereotopic atoms, groups and faces, stereospecific and stereo selective 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 phosphours.

Unit-II

(a) Reaction Mechanism : Structure and Reactivity : Type of mechanisms, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammonds' Postulates, 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 radical, carbenes and nitrenes. Effect of structure on 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.

(b) Aliphatic Nucleophilic Substitution : The SN^1 , SN^2 , mixed SN^1 and SN^2 and SET mechanisms, neighbouring group participation by Sigma and Pi bonds. Anchimeric assistance. Classical and nonclassical carbocations, phenonium ions norbornyl system, common carbocations rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN mechanisms. 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, ambidentate nucleophile, regioselectivity.

Unit-III

(a) Aliphatic Electrophilic Bimolecular mechanism SE^1 and SE^2 the SE mixed mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

(b) 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. Vilsmeier reaction, Gattermann-Koch reaction.

(c) Aromatic Nucleophilic substitution : the SN^Ar , SN , Benzyl and SRN mechanisms. Reactivity- effect of substrate structure, leaving group and

Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution.

Determination of pKa of an indicator (methyl red) in (i) aqueous and (b) micellar media.

Characterization of the complexes by electronic and IR spectral data.

Estimation of Pb^{2+} and Cd^{2+}/Zn^{2+} and Ni^{2+} by polarography.

Determination of dissolved oxygen in aqueous solution of organic solvents.

Interdisciplinary Green chemistry experiment (should be performed where more than one special paper is being taught)
Preparation and characterization of Biodiesel from vegetable oils (Biodiesel may be prepared from different oils, catalysts and determination of their physical properties viz viscosity, surface tension, flash point

Experiments related with computational and virtual chemistry may be designed and performed.

(F) Electronics:
This lab course will have theory as well as practical and the lectures shall be delivered during lab hours.

Basic Electronics:
Notations used in the electronic circuit, study of electronic compounds and colours codes, conversion of chemical quantities into electronic quantities transducer, illustration with electrodes, thermocouples and thermistors.

Passive components;
Resistors capacitors and inductors with some emphasis on solid state properties of materials. Net works of resistors Thevenin's theorem super position theorem loop analysis, R.C. circuits in NQR Spectroscopy, Mossbauer spectroscopy cyclic voltametry and in power supplies as circuits.

Active Components :
Introduction to ordinary diodes and Zener diodes with some emphasis on p-n junction as a solid state property. Use of diodes as rectifiers clipping and clamping circuits power supplies.

Transistor:
An extension of p-n junction of pnp and npn transistors Characteristics of transistors ,hybrid parameter, transistors circuits as amplifiers, high impedance (preamplifier) circuits, darlington pairs differential amplifiers.

Operational Amplifiers
Ideal Characteristics; inverter, summer, integrator, differentiator, voltage follower, illustrative use of operational amplifiers. Introduction to fourier transformation in instrumentation

List of Experiments in Electronics
(Do at least five experiments from this section)

1. (a) To plot the diode characteristics and find its dynamic resistance and cut in voltage.

8. To determine the degree of hydrolysis and hydrolysis constant of salts (e.g. CH_3COONa , NH_4Cl)
9. Determination of hydrolysis constant of aniline hydrochloride.
10. Titration of a solution of a salt of a weak base and strong acid, say NH_4Cl
- (B) Experiments based on Potentiometric and pH measurements:**
- Potentiometric and pH metric titrations: Acid-base, oxidation-reduction and complex salts.
 - Titration of a mixture of HCl and CH_3COOH and hence the composition of the mixture.
 - Titration of a mixture of CH_3COOH and CH_3COONa and to determine the dissociation constant of the acid.
 - To determine the ionization constants of a polybasic acid (H_3PO_4).
 - To determine the solubility and solubility Product of AgCl , AgBr and AgI .
 - To determine the hydrolysis constant of aniline hydrochloride.
 - Determine the composition of a given mixture containing KCl and KClO_4 .
 - Determination of acid, and basic dissociation constants of an amino acid, and hence the iso-electric point of the acid.
 - To determine the solubility product of silver halide (AgCl)
 - Determination of Ionic product of water.
- (C) Experiments based on Kinetics:**
- To study the nature of salt effect on $\text{S}_2\text{O}_8^{2-}$ -I reaction and conclude the nature of the species in the slow step.
 - To investigate the inversion of cane sugar in presence of an acid. Determine the energy of activation of the reaction.
 - To study the kinetics of hydrolysis of ethyl acetate by NaOH at two temperatures by conductance measurement, and hence the energy of activation of the reaction.
 - To study the kinetics of decomposition of the complex formed between sodium sulphide and sodium nitro prusside.
 - To study the inversion of cane sugar in presence of HCl and H_2SO_4 and hence determine the relative strength of the acids.
 - To investigate the autocatalytic reaction between potassium permanganate and oxalic acid.
- (D) Experiments based on spectrophotometry**
- To determine the composition of binary mixture containing $\text{K}_2\text{Cr}_2\text{O}_7$ and KMnO_4 using a spectrophotometer.
 - Test the validity of Beer-Lambert's law and determine the concentration of Glucose solution.
 - To determine the concentration of Metal ions by spectrophotometric titration with EDTA (Copper, Nickel and iron)
 - Determination of ionisation constant of bromophenol blue.
 - To determine phosphate concentration in a soft drink.
- (E) Miscellaneous Experiments**
- Determination of partial molar volume of solute (KCl) and solvent in a binary mixture.
- attacking nucleophile. The Von Richter, Sommelet-Hauser and Smiles rearrangements.
- (d) Free Radical Reactions :** Types of free radical reactions, free radical substitution mechanisms, 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.
- Unit-IV**
- (a) Addition to Carbon-Carbon Multiple Bonds :** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction sharpless asymmetric epoxidation.
- (b) Addition to carbon-Hetero Multiple Bonds :** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compound, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reactions. Mechanism of condensation reactions, involving enolates. Aldol, Knoevenagel Calsien, Mannich Benzoin, Perkin and Stobee reactions. Hydrolysis of esters and amides ammonolysis of esters.
- Unit-V**
- (a) Elimination Reactions :** The E_2 , E_1 and E_1cb mechanisms and their spectrum. Orientation of the double bond, reactivity effects of substrate structures, attacking base, the leaving groups and the medium. Mechanism & orientation in pyrolytic elimination.
- (b) Pericyclic Reactions :** Molecular orbital symmetry, frontier orbital of ethylene, 1, 3-butadiene, 1,3, 5 hexatriene and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements – suprafacial and antarafacial shifts of H sigmatropic shifts involving carbon moieties, 3,3, - and 5,5- sigmatropic rearrangements. Claisen, cope and azab-cope rearrangements. Fluxional tautomerism. Ene reaction.
- Books Suggested :**
- Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley.
 - Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
 - 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, RT Morrison and R.N. Boyd, Prentice Hall.
6. Modern Organic synthesis, R.O.C. Norman and J.M. Coxon Blackie Academic & Professional.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Pericyclic Reactions, S.M. Mukherji, Macmillian India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh Macmillian.
10. Stereochemistry of Organic Compounds, P.S. Kalasi, New Age International.

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

E. Spectrophotometric (UV/VIS) Estimations (Any Three)

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeins

Instructions to Examiners

Five exercises are to be given, selecting one from each section from A to E.

Marking Scheme Exercise	Marks
Exercise No. 1 (from section A)	35
Exercise No. 2 (from section B)	30
Exercise No. 3 (from section C)	15
Exercise No. 4 (from section D)	15
Exercise No. 5 (from section E)	15
Viva	10
Record	10
Project Work & Seminar	20
Total	150

Note: Seminar Marks for seminars will be awarded by panel of examiners / experts (which will conduct seminars) constituted internally by Head of the department which will be hand over it to the board of examiners. It is advised to conduct two seminars one in the mid of the session and one at the end of the session.

PAPER-III CH-403 PHYSICAL CHEMISTRY

Time : 3 Hours **Max. Marks :75**

Unit-I

Quantum Chemistry

(a) **Introduction to Exact Quantum Mechanical Results :** The Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotator, the hydrogen atom.

(b) **Approximate Methods :** The variations theorem, linear variation principle. Perturbation theory (first order an non- degenerate). Application of variation methods and perturbation theory to the Helium atoms.

(c) **Angular momentum :** Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operations, addition of angular, momenta, spin, antisymmetry and Pauli exclusion principle.

(d) **Electronic Structure of Atoms :** Electronic configuration, Russel Saunders terms and coupling schemes, Slater- Condon parameters, term separation energies of the Pn configuration, term separation energies for the dn configurations, magnetic effects- spin orbit coupling and Zeeman splitting, introduction to the methods of self consistent field, the virial theorem.

(e) **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-II

Thermodynamics

(a) **Classical Thermodynamics :** Brief resume of concepts of laws of thermodynamics, free energy potential and entropies. Partial molar properties; practical molar free energy, partial molar volume and partial molar heat content and their significances.

M.SC. (FINAL) CHEMISTRY PRACTICAL

Time: 14 Hours **Max. Marks: 150**
(Spread in 2 Days) (Including 20 Marks for Project Work & Seminar)

PHYSICAL CHEMISTRY

A. Experiments based on Conductivity measurements:

1. Conductometric Titration: Acid-base, Precipitation and complex salts.
2. To determine the equivalent conductance of a weak electrolyte at different concentrations and hence test the validity of Ostwald's dilutions law. Also determine the dissociation constant of the weak electrolyte.
3. To determine the equivalent conductance of a strong electrolyte at several dilutions, and hence verify the Onsager equation.
4. To determine the equivalent conductance of a weak electrolyte at infinite dilution using the Kohlraush law.
5. To determine the solubility of a sparingly soluble salt in water by conductance measurement.
6. To determine the basicity of an organic acid by conductometric measurement.
7. To determine the composition of a mixture of acetic acid and hydrochloric acid by conductometric titration.

ORGANIC CHEMISTRY

Qualitative Analysis

(A) Separation, purification and identification of the components of mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid) using TLC for checking the purity of the separated compounds. Chemical analysis.

(B) Multi-Step Synthesis of Organic Compounds (Any Four)

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

a. Photochemical reactions

Bebzophenone benzpinacol benzpinacolone

b. Beckmann rearrangement : benzanilide from benzene

Benzene Benzophenon Benzophenone oxime Benzanilide

c. Benzilic acid rearrangement Benzilic acid from benzoin.

Benzoin Benzil Benzilic acid

d. Synthesis of heterocyclic compounds Skraup synthesis : preparation

of quinoline from aniline Fisher-Indole synthesis : preparation of 2-phenylindole from phenylhydrazine.

e. Enzymatic synthesis- enzymatic reduction ; Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S(+) ethyl-3-hydroxybutanoate and determine its optical purity.

f. Biosynthesis of ethanol from sucrose.

g. Synthesis using microwaves Alkylation of diethyl malonate with benzyl chloride.

h. Synthesis using phase transfer catalyst.

i. Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.

j. Green Synthesis -1. Solvent free Aldol condensation and 2. Benzoin condensation with thiamine as a catalysts instead of cyanide

NOTE —Other similar synthesis of three steps.

C. Extraction of Organic Compounds from Natural Sources (Any Five)

1. Isolation of caffeine from tea leaves.

2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).

3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).

4. Isolation of nicotine dipicrate from tobacco.

5. Isoation of cinchonine from cinchona bark.

6. Isolation of piperine from black pepper.

7. Isolation of lycopence from tomatoes.

8. Isolation of β -carotence from carrots.

9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid.

10. Isolation of eugenol from cloves.

11. Isolation of (+) limonine from citrus rinds.

D. Spectroscopy

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 coefficient, ionic strength. Application of phase rule to three component systems; second order phase transitions.

(b) Statistical Thermodynamics : Concept of distribution, thermodynamics probability and most probable distribution. Ensemble averaging, postulates of ensemble and everaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions translational, rotational, vibrational and electronic partition functions, calculating 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 applications to metal. Bose-Einstein Statistics-distribution law and applications to helium.

(c) Non-Equilibrium Thermodynamics : Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equation 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, electro kinetic phenomena diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Unit-III

Chemical Dynamics :

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 barrier less chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit-IV

Surface Chemistry

(a) Adsorption ; Surface tension, capillary action, pressure difference: across curved surface (laplac-equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption, isotherm, estimation of surface area (BET

equation), Surface films on liquids (Electro-kinetic phenomenon) Catalytic activity at surfaces.

(b) **Micelles** : Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, 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.

(c) **Macromolecules** : Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Unit-V Electrochemistry

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions, Debye-Huckel-Jerum mode.

Thermodynamics of electrified interface equations, Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interface. Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan model.

Over potentials, exchange current density, derivation of Butler-Volmer equations, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Semiconductor in terfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. effect of light at semiconductor solution interface.

Electro catalysis-influence of various parameters. Hydrogen electrode Bioelectrochemistry, threshold membrane phenomena, Nemst-Planck equation, Hodge-Huxley equations, core conductor models, electrocardiography.

Polarography theory, Ilkovic equation; half wave potential and its significance.

Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Books Suggested:

- Physical Chemistry, P.W. Atkins, ELBS.
- Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- Quantum Chemistry, Ira N. Levine, Prentice Hall.
- Coulson's Valence, R. McWeeny, ELBS.
- Chemical Kinetics, K.J. Laidler, McGraw Hill.
- Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
- Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
- Modern Electrochemistry Vol. 4 and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
- Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Easter.

a. Manganese/ Chromium/ Vanadium in steel sample.

b. Nickel/molybdenium/tungsten/vanadium/uraniumby extractive spectrophotometric method.

c. Fluoride/nitrite/phosphate.

(ii) Determination of Metal Ligand ratio & Stability constant.

a. Iron-phenanthroline complex : Job's Method of continuous variations.

b. Zirconium-Alizarin Red-S complex : Mole-ratio method.

c. Copper-Ethylene diamine complex : Slope-ratio method.

C. Flame Photometric Determinations (Any Three)

a. Sodium and potassium when present together

b. Lithium/calcium/barium/strontium.

c. Cadmium and magnesium in tap water.

d. Sulphate.

e. Phosphate.

f. Silver.

D. Chromatographic Separations (Any Three)

a. Cadmium and Zinc.

b. Zinc and Magnesium

c. Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of Rf values.

d. Separation and identification of the sugars present in the given

mixture of glucose, fructose and sucrose by paper chromatography and raphy and determination of Rf Values.

Instructions to Examiners

Five exercises are to be given, selecting two exercises from section A and One exercise from each section from B to D.

Marking Scheme

Exercise

Marks

Exercise No. 1 (from section A)

20

Exercise No. 2 (from section A)

15

Exercise No. 3 (from section B)

25

Exercise No. 4 (from section C)

25

Exercise No. 5 (from section D)

25

Viva

10

Record

10

Seminar & project work

20

(Best of two seminars)

Total

150

Note: Seminar Marks will be awarded by panel of examiners / experts (which will conduct seminars) constituted internally by Head of the department which will be hand over it to the board of examiners. It is advised to conduct two seminars one in the mid of the session and one at the end of the session.

M.SC. (FINAL) CHEMISTRY PRACTICAL

Time: 14 Hours

Max. Marks: 150

(Spread in 2 Days) (Including 20 Marks for Project Work & Seminar)

- hexachloro-plumbate $(\text{NH}_4)_2 \text{PbCl}_6$.
8. Hexa-bis (4-Nitrophenox cyclotriphosphazene.)
9. Synthesis of trichlorodiophenylantimony (V) hydrate Synth., 1985, 23, 194.
10. Sodium tetrathionate $\text{Na}_2\text{SO}_4 \cdot 8\text{H}_2\text{O}$.
11. Metal complexes of dimethyl sulfoxide (lr); $\text{CuCl}_2 \cdot 2 \text{DMSO}$, $\text{PbCl}_2 \cdot 2 \text{DMSO}$, $\text{RuCl}_2 \cdot 4 \text{DMSO}$. J. Chem. Educ., 1982, 59, 57.
12. Synthesis of metal acetylacetonate, Magnetic moment, IR, NMR. Inorg. Synth., 1957, 5, 130, 1963, 1, 183.
13. Bromination of $\text{Cr}(\text{acac})_2$. J. Chem. Edu., 1986, 63, 90.
14. Magnetic moment of $\text{Cu}(\text{acac})_2 \cdot 2\text{H}_2\text{O}$.
15. Separation of optical isomer of cis- $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$. J. Chem. Sec., 1960, 43, 69.
16. Ion exchange separation of oxidation state of vanadium. J. Chem. Educ., 1980, 57, 316, 1978, 55, 55.
17. Determination of Cr (III) complexes $[\text{Cr}(\text{H}_2\text{O})_6 \text{NO}_3 \cdot 3\text{H}_2\text{O}$, $[\text{Cr}(\text{H}_2\text{O})_4 \text{Cl}_2] \text{Cl} \cdot 2\text{H}_2\text{O}$, $[\text{Cr}(\text{en})_3] \text{Cl}_3$, $\text{Cr}(\text{acac})_3$ Inorg. Synth., 1972, 13, 184.
18. Preparation of N. N bis (salicyldehyde) ethylenediamine, salen H_2 , C₆O (Salen) J. Chem. Educ., 1977, 54, 443, 1973, 50, 670. Determination of O₂ absorption by Co (salen) Acct. Chem. Res., 1975, 8, 384. Reaction of Oxygen adduct with CHCl_3 (deoxygenation).
19. Preparation of Fe (II), chloride (use it as Friedal- Craft chlorination source J. Org. Chem. 1978, 43, 2423, J. Chem. Edu., 1984, 61, 645, 63, 361.
20. Reaction of Cr. (III) with a multidentate ligand a kinetics experiments (visible spectra Cr-EDTA complex) J.A.C.S., 1953, 75, 5670.
21. Preparation of $[\text{Co}(\text{phenanthroline}-5,6\text{-quinone})]$. J. Chem Soc A, 1970 447, J. Chem Edu. 1977, 54, 710.
22. Preparation and use of Ferrocene. J. Chem. Edu., 1966, 43, 73, 1976, 53, 730.
23. Preparation of copper glycine complex-cis and trans bis glycinato cooper (II). J. Chem. Soc. Dalton, 1979, 1901, J. Chem. Edu., 1966, 43, 73, 1976, 53, 730.
24. Preparation of Phosphine Ph_3P and its transition metal complexes.
25. Conversion of p-xylene to terephthalic acid catalyzed by CoBr_2 (homogeneous catalysis).
26. Preparation of any other Inorganic Compound of more difficult type.
27. Green Synthesis of fluorescent isomers of tris (8-hydroxyquininoloto) aluminium (III)
28. Green Synthesis of Synthesis of Bis (acetylacetonato) Manganese (III)
29. Green Synthesis of any organometallic compound
30. Green Preparation of biodiesel
31. Preparation of nanoparticles of metals or metal compounds
32. Experiments related with computational and virtual chemistry may be designed and performed.
- B. Spectrophotometry**
- (i) Estimation
- Paper-IV : CH-404 ANALYTICAL CHEMISTRY**
Time: 3 Hours **Max. Marks : 75**
- Unit-I**
- (a) **Drug analysis** - Principles of determination of functional groups; Protocols for the analysis of standard drugs. Food standards and Specifications Anti microbial agents / Class I and Class II preservatives as per PFA Act.
- (b) **Soil and water analysis**
- Unit II**
- Electroanalytical Methods:**
- (a) **Potentiometry/ pH- metry:** Basic principles, instrumentation, experimental technique, electrodes-reference, indicate-ion sensitive and recent advances in potentionmetry and application.
- (b) **Conductometry:** Basic Principle, instrumentation, experimental technique, Low & High frequency titration.
- (c) Voltammetry of Alternating Current (AC), Linear potential sweep (DC) cyclic potential swep voltammetry (CV) and strpping (Anodic & Cathoding) Analysis.
- (d) **Thermal Analysis Methods:** Basic principles, instrumentation, experimental technique of Differential Scanning Calorimetry and Differential analysis, Thermo gravimetry, Thermo mechanical analysis, Dynamic mechanical analysis, thermometric titrimetry and direct injection Enthalpimetry.
- Unit-III**
- (a) **Atomic Spectroscopy :** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.
- 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.
- (b) **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.
- Photoacoustic Spectroscopy : Basic principles of photoacoustic spectroscopy (PAS), PAS-gases and condensed systems, chemical and surface applications.
- Unit-IV**
- Theory Principle, experimental techniques and application of IR, Raman, Microwave and NMR spectroscopy. Special emphasis on FTIR and FTNMR.
- Unit-V**
- (a) **X-Ray Diffraction :** Bragg condition, Miller indices, Laue methods, Bragg method Debye Scherrer method of X-ray structural

analysis of crystal, 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.

(b) **Electron Diffraction** : Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules, Low energy electron diffraction and structure of surfaces.

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

Books Suggested:

1. Modern Spectroscopy, J.M. John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer 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, R. Chang, McGraw Hill.
7. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
8. Theory and Applications of UV Spectroscopy, H.H. Jaffeand M. Orchin,
9. Introduction to Photoelectron Spectroscopy, P.K; Ghosh, John Wiley.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Carrington and AD. Maclachalan, Harper & Row.

M.Sc. (PREVIOUS) CHEMISTRY PRACTICAL

Time: 14 Hours (Spread over Two days)

Max. Marks : 150 Min.Marks :54

Identification of safety symbols

Qualitative Analysis:

- (a) Analysis of Inorganic mixture containing eight radicals, out of which at least one should be less common metal ion
- (b) Insolubles-oxides, sulphates and halides. Interfering radicals

Quantitative Analysis

- (c) separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.
- (d) Determination of DO, COD and BOD of water sample.

Chromatography:

13. M.S. Creos and Morr, Environmental Chemical Analysis, American publication(1988)
14. A.K. De, Environmental Chemistry, New Age International publishers.Moghe and
15. Ramteke, Water and waste water analysis : (NEERI)
16. A.C. Stern, Air pollution: Engineering control vol.IV(AP)
17. P.N.Cheremisinoff and R.A.Young, Air Pollution controland Design.Hand Book Vol.I&II (Dekker)
18. B.K.Sharma, Industrial Chemistry.
19. S.P.Mahajan, Pollution Control in Process Industries.
20. R.A.Horne, Chemistry of our Environment.
21. Ruzica and Stary, Substochiometry in Radiochemical Analysis. Pergamon.
22. Ladd and Lee, Radiochemistry.
23. Clerk, Handbook of Radiochemical methods
24. Hillebrand Lhundel Bright and Hoffman, Applied Inorganic Analysis, John Wiley.
25. Snell and Biffen, Commercial Methods of Analysis.
26. P.G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
27. Allan Cury,Irvins Sunshine,Forensic Analysis, Academic Press Publications.
28. Karamer Twig: Quality control for food industry (AVI)
29. G. F. Longonan: the analysis of detergents and detergent products (JW)
30. A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
31. Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
32. Aubert and Pintes, Trace Elements in Soils.
33. Bear, Chemistry of Soil.
34. Hauson, Plant Growth Regulators, Noyes.

M.Sc. (FINAL) CHEMISTRY PRACTICAL

Time: 14 Hours

Max. Marks: 150

(Spread in 2 Days) (Including 20 Marks for Project Work & Seminar)

INORGANIC CHEMISTRY

Preparation of selected inorganic compounds and their study by IR, electronic spectra, Mossbauer, ESR magnetic susceptibility measurements, Handling of air and moisture sensitive compounds involving vacuum lines.

A. Preparation (Minimum Seven)

1. Sodium amide, Inorg Synth., 1946, 2, 128.
2. Synthesis and thermal analysis of group II metal oxalatehydrate. J. Chem. E., 1988, 65, 1024.
3. Atomic absorption analysis of Mg. and Ca.
4. Trialkoxyboranes-Preparation, IR and NMR spectra.
5. PhBCl₂ dichlorophenylborane-Synthesis in vacuum line.
6. Preparation of Tin (IV) Iodide, Tin (V) chloride and Tin (II) iodide. Inorg. Synth., 1953m 4, 119.
7. Relative stability of Tin (V) and Pb (IB). Preparation of ammonium hexachlorostannate (NH₄) SnCl₆ ammonium

solvent extraction, oxidation method and microbiological treatment.

Unit-IV Food and Forensic Analysis

(a) Food analysis: Moisture, ash, crude protein, fat, crude fiber, carbohydrate, calcium, potassium, sodium, and phosphates, food adulteration – common adulteration 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 organo – phosphates, thin layer chromatography for identification of chlorinated pesticides in food products.

(b) Special features of Forensic analysis:- sampling, sample storage, sample dissolution, classification of poisons, Lethal dose, significance of LD 50 and LC 50.

Unit -V Organic Industrial Analysis:-

(a) Analysis of oils, fats, soaps and detergents: Introduction to natural fats and oils, Analysis of oils and fats: Softening point, Conger point, Titre point, cloud point, Iodine, Saponification, acid, hydroxyl, R-M and Polenske value, Elaiden test. Introduction to soaps, analysis of soap (saponifiable, unsaponifiable) and for unsaponified matter in soaps, Estimation of free alkali and phenol in soap. Classification of detergents (in Brief): Analysis of active ingredients from detergents (methylene blue and Hyamine-1622 method); Estimation of CMC, Chlorides, total phosphates etc.

(b) Analysis of dyes and paints: Types of dyes, and their analysis. Composition and analysis of paints, determination of volatile and non-volatile constituents, flash points, separation of pigments, estimation of binders and thinners.

Reference Books:

1. F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II (D. Van Nostrand Comp.)
2. I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
3. F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
4. Riech: Outline of Industrial Chemistry.
5. K. H. Buchel: Chemistry of Pesticides (John Wiley)
6. Nichollas: Aids to the Analysis of foods and Drugs.
7. A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)
8. S. Ranganna: Handbook of analysis and quality control for fruits and vegetable products (McGraw Hill)
9. Ramalu: Analysis of pesticides
10. Bassett, Denney-Jeffers and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis, (5th edition).
11. A.K. De : Standard Methods of Waste and Waste water analysis.
12. S.M. Khopkar, Environmental Chemistry ; Environmental pollution analysis.

separation of cations and anions by

- (a) Paper chromatography
- (b) column chromatography-ion exchange.

Preparations

Preparations of selected inorganic compounds and their studies by I.R., electronic spectra, Mossbauer, E.S.R and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds. Study of instruments related to various techniques described in syllabus.

- (1) VO (acac)
- (2) TiO (C₉H₈NO) 2H₂O
- (3) cis-K [Cr (C₂OH)₂(H₂O)₂]
- (4) Na[Cr(NH₃)₂(SCN)₄]
- (5) Mn(acac)₃
- (6) K₂[Fe(C₂O₄)₃]
- (7) Prussian blue, Turnbull's Blue
- (8) [Co(NH₃)₆][Co(NO₂)₆]

(9) Green Synthesis (a) Synthesis of Bis (acetylacetonato) Copper (II)

(b) Synthesis of Bis (acetylacetonato) Iron (III)

(10) Nanoparticles synthesis – Zn/ZnO/Ag/MnO etc.

Virtual Chemistry Experiments

Experiments related with molecular modeling, virtual synthesis, virtual titrations, virtual chromatography etc. can be performed.

ORGANIC CHEMISTRY

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis (Any Five)

- 1- Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
 - 2- Oxidation : Adipic acid by chromic acid oxidation of cyclohexanol.
 - 3- Grignard reaction : synthesis of triphenyl methanol from benzoic acid.
 - 4- Aldol condensation : Dibenzal acetone from benzaldehyde.
 - 5- Sandmeyer reaction : p chlorotoluene from p-toluidine.
 - 6- Acetoacetic ester condensation : synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
 - 7- Cannizzaro reaction : 4-chlorobenzaldehyde as substrate.
 - 8- Friedel craft's reaction : b. Benzoyl propionic acid from succinic anhydride and benzene.
 - 9- Aromatic electrophilic substitutions : synthesis of p-nitroaniline and b-bromoaniline.
- The products may be characterized by spectral techniques.

Quantitative Analysis:

- 1- Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
- 2- Estimation of amines / phenols using bromate bromide solution /or acetylation method.
- 3- Determination of Iodine and Saponification values of an oil sample.

Physical chemistry

Number of hours for each experiment : 3-4 hours. A list of experiments under different headings is given below typical experiments are to be selected from each type. Students are required to perform at least 10 experiments.

Error Analysis and Statistical Data Analysis:

Errors, type of errors, minimization of errors, error distribution curves, precision, accuracy and combination, statistical treatment for error analysis, student 'T' test null hypothesis, rejection criteria F& Q test; linear regression analysis, curve fittings,

Calibration of volumetric apparatus, burette, pipette and standard flask.

Absorption.

To Study surface tension-concentration relationship for solutions (Gibb's equations)

Phase Equilibria

(i) Determination of congruent composition and temperature of a binary system (e.g.) diphenylamine- benzophenone system)

(ii) Determination of transition temperature of a given salt (e.g., CaCl_2) conductometrically.

(iii) To construct the phase diagram for three component system (e.g.) chloroform-acetic acid-water).

Chemical Kinetics :

(i) Determination of the effect (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.

(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as iodine clock reaction.

(iv) Flowing clock reactions (Ref. :Experiments in Physical chemistry by Showmaker).

(v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)

(iv) Oscillatory reaction.

Solutions

(i) Determination of molecular weight of non- volatile and non- electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

(ii) Determination of the degree of dissociation of weak electrolyte and to study of deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry :

A- Conductometry :

(i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

8- Basic Concepts of Analytical Chemistry, S.M. Kholkar, Wiley Eastern.

9- Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle Prentice Hall.

Group-D

PAPER : X- B CH-510 APPLIED ANALYTICAL CHEMISTRY

Time : 3 Hours

Max. Marks : 75

Unit-I

(a) Pharmaceutical Analysis:- Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests for impurities like, Pb, As, Fe, moisture, chlorides, sulfates, Boron, free halogen, selenium etc. Analysis of some commonly used drugs like sulfadiazole, antihistamines, barbiturates, vitamins (A, B₆, C, E, K) etc

(b) Clinical Analysis : Composition of blood, collection, and preparation of samples, clinical analysis – serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulin, barbiturates, acidic and alkaline phosphates, Immunoassay, principles of radio immunoassay, 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 spectrophotometric analysis

Unit-II: Analysis of soil, fertilizers and Fuels

(a) Analysis of soil and fertilizers: Moisture, pH, total nitrogen, phosphorous, silica, lime, Magnesia, Manganese, sulfur & alkali salts. Method of soil analysis, soil fertility its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers.

(b) Fuel Analysis:- Solid, liquid and Gas Fuels:- Solid Fuels: ultimate and proximate analysis, heating values, grading of coal. Liquid fuels: flash points, aniline point, octane number and carbon residue, Gaseous fuels: producer gas and water gas – calorific value.

Unit-III: Environmental Analysis

(a) Environment - its characteristics and Classification: Metallic and non-metallic pollutants, Cr, Hg, Pb, Cd, Cu, As etc. Their physiological manifestation, source, analysis and control of inorganic compounds. Chemistry of Air pollutants, Characterization. Source, methods of analysis of air pollutants; CO, CO₂, NO_x, NH₃, H₂S, SO₂, etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen (DO) Chemical oxygen demand (COD) Biochemical oxygen demand (BOD) and their measurements and significance in waste water treatments, Threshold odour number.

(b) Industrial waste Water analysis for organic and Inorganic Constituents:

Chemistry of odour and its measurements Sewage and sludge analysis. Treatment, disposal and source of phenolic residue, Analytical methods, treatment by using stream. Gas stripping, ion exchange,

(e) Electron Microscopy: Types (TEM, SEM, REM and LVEM), sample preparation and application in life sciences, industries and research Scanning and Transmission Electron Microscopy

UNIT-III

Spectrophotometric Methods:-

(a) UV-Vis Spectrophotometry:- Theory, instrumentation, experimental technique for determination, differential and derivative spectroscopy, photometric titrations.

(b) Fluorescence & Phosphorescence Spectrophotometry :Basic principles, instrumentation, experimental technique and important application.

(c) Atomic Absorption and Flame Emission Spectroscopy(AAS & FES): Elementry theory, Instrumentation for atomic absorption & Reame emission spectroscopy, experimental technique and important applications. Comparison of AAS& FES.

(d) Fluorimetry, Nephelometry & Turbidimetry: Basic principles, instrumentations, experimental technique & important applications.

UNIT-IV

Chromatography: Basic principles, Instrumentation, experimental technique and important application of following-

(a) Thin layer chromatography(TCL), paper, column, Ion-Exchange chromatography

(b) Gas Chromatography (GC), Gas Liquid Chromatography (GLC), High performance liquid chromatography (HPLC).

UNIT-V

Ceramic analysis and Instrumentation

(a) Description and classification of various minerals based on their chemical compositions, Physical properties and occurrence.

(b) Study in detail of raw materials used in glass, Refractories, White wares, Potteries and Cement

(c) Chemical characteristic of raw materials of alkali and alkaline earth elements, Silica, Silicates, Alumina, Aluminates, Titania, Zirconia and and zircon,

Chromatography : Introduction, Paper and thin layer chromatography, Liquid chromatography, Types of liquid chromatography, Column and detection systems: Differential thermal analysis (DTA) and thermo gravimetric analysis (TGA) with suitable examples.

Books Suggested :

1- Analytical Chemistry, G.D. Christian, J. Wiley.

2- Fundamentals of Analytical Chemistry, D.A. Skoog,, D.M. Westand F.J. Holler, W.B. Saunders.

3- Analytical Chemistry – Principles, J.H. Kennedy, W.B. Saunders.

4- Analytical chemistry – Principles and techniques, LG. Hargis, Prentice Hall.

5- Principles of Instrumental Analysis, D.A. Skoog, 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.

(ii) Determination of the degree of dissociation of weak electrolyte and to study of deviation from idealbehaviour that occurs with a strong electrolyte.

(iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.

(iv) To study the effect of solvent on the conductance of AgNO₃, acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO DMF dioxane, acetone, water) and to test the validity of Debye Huckels limiting law.

B- Potentiometry / pH metry:

(i) Determination of strengths of halides in a mixture potentiometrically.

(ii) Determination of the valence of mercurous ions potentiometrically.

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

(iv) Determination of temperature dependence of EMF of a cell.

(v) Determination of the formation constant of sliver- ammonia complex and stoichiometry of the complex potentiometrically.

(vi) Acid-base titration in a non-aqueous media using a pH meter.

(vii) Determination of activity and activity coefficient of electrolytes.

(viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

(ix) Determination of the dissociation constant of monobasic/ dibasic acid by Albert - Serjeant method.

(x) Determination of thermodynamic constants, DG, DS and DH for the reaction by e.m.f. method.

Polarimetry:

(i) Determination of rate constant for hydrolysis/ inversion of sugar using a polarimeter.

(ii) Enzyme - kinetic - inversion of sucrose.

Computational chemistry

Experiments on molecular modeling, computational chemistry, metal-drug, metal-protein interaction etc. can be performed.

Reference Books:

1- Vogel's Textbok of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffrey and J. Mendham, ELBS.

2- Experiments and Techniques in Organic Chemistry, D.P. Pasto, C Johnson and M. Miller, Prentice Hall.

3- Macroscale and Microscale Organic Experiments, K.L. Williamson D.C. Health.

4- Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.

5- Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell,

6- Practical Physical chemistry, A.M. James and F.E. Porichard, Longman.

7- Findley's Practical Physical Chemistry, B.P. Levitt, Longman.

8- Experimental Physical Chemistry R.C. Das and B. Behera,

9- Green Chemistry : An experimental study, R.K. Sharma, N. Bhojak, I.T. Sidhwani and M.K. Choudhary

INSTRUCTIONS OF THE EXAMINERS.**M.Sc. (Previous) Chemistry Practical.****Inorganic Chemistry.****Qualitative and Quantitative Analysis:-**

(i) Analysis of mixture containing 8 radicals including two radicals of rare elements.

OR

Separation and determination of two metal ions Cu- Ni, Ni-Zn, Cu Fe etc. involving volumetric and gravimetric method.

25

(ii) Separation of cations and anions by paper chromatography or column chromatography.

OR

Preparation of one selected inorganic compound and its study by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements.

15

Organic Chemistry.

(i) Qualitative Analysis Separation, purification and identification of the components of binary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests, IR spectra to be used for functional group determination.

OR

organic synthesis perform one of the 9 organic synthesis as mentioned in the syllabus and product may be characterized by spectral techniques.

25

(ii) Quantitative Analysis Perform one the of four quantitative analysis.

(a) Estimation of amines / phenols using bromate- bromide method or acetylation method.

(b) Determination of the percentage or number of hydroxyl groups in organic compound by acetylation method.

15

(c) Determination of iodine and saponification values of an oil sample.

(d) Determination of DO, COD and BOD water sample.

20+20

Physical Chemistry

Perform any two physical experiments (both experiments should not be from same topic).

A list of experiments under different headings is given in the syllabus. Typical experiments are to be selected from each types. Students are required to perform at least 10 experiments in the class. Identification of safety symbols to be performed in Record and shall be examined during viva. The candidate must perform at least four experiments based on four different instruments like = Uv-vis spectrophotometer, FTIT, Conductometer, Colorimeter, pH meter, Flame photometer, Polarimeter, Potentiometer and / or any other sophisticated instrument.

Spotting

(b) **Density functional theory** : Derivation of Hohenberg- Kohn theorem, kohn sham formulation, N- and V- representabilities; review of the performance of the existing local (e.g. slater Xa and other methods) and non local functions, treatment of chemical concepts with the density functional theory.

Book Suggested :

- 1- Computational Chemistry, A.C. Norris, John Wiley.
- 2- Computer Programming in FORTRAN 77, R Rajasthan, Prentice Hall.
- 3- Numerical Analysis, CE. Frogberg, Macmillan.
- 4- Numerical Analysis-A Practical Approach, M.J. Meron, John Wiley
- 5- Numerical Methods for scientists and Engineers H.M. Antia Tat Mcgrow Hill.
- 6- Modern Quantum Chemistry N.S. Ostlund and A. Szabo, McGraw Hill.
- 7- Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, academic Press.
- 8- Density Functional Theory of Atoms and Molecules, RG Parrand W Yang, Oxford.
- 9- Exploring Chemistry with Electron Structure Methods, JB. Foresman and E. Frish Gaussian Inc.
- 10- Semi-Empirical MO Theory, J. Pople and D.L. Beveridge.

Group-D**PAPER : X-A CH- 509 ANALYTICAL CHEMISTRY****Time : 3 Hours****Max. Marks : 75****UNIT-I****General consideration in analysis-**

(a) Instrumental Methods- Classification of techniques, important consideration, measurement of data sensitivity and detection limit, Noise, Signal to noise ratio, Accuracy and instrument calibration, Evaluation results by statistical methods.

(b) Computer Aided Analysis: Computer organization -Software & Hardware, interfacing computers in instruments.

(c) Process control & Laboratory Analyzer: Industrial process analyzers- Infrared, Oxygen, potentiometric and gas-chromatographic, online process control, Automatic chemical analyzer and element (C,H,N,O) analyzer.

UNIT-II**Spectral methods of Analysis-**

(a) Raman Spectroscopy- Theory, Instrumentation, experimental technique and structural analysis.

(b) Infrared Spectroscopy, Sample handling, Instrumentation, experimental technique, qualitative and quantitative analysis, FT-IR & NIR,

(c) Mass-Spectrometry:- Mass, spectrometry, Sample flow, inlet sample system, ionization methods, mass analyzers, ion-collection system, experimental technique and correlation of Mass spectra with molecular structure.

(d) X-Ray Spectra:- Instrumentation, experimental technique of X-Ray analysis-Direct, X-ray Diffraction (XRD), Absorption(XRA) & Fluorescence (XRF)

(iv) **Interpolation** : Newton forward and backward difference, central differenced formulae, Lagrange and Hermite interpolation, polynomial wiggle problem.

(v) **Numerical differentiation** : Solutions of simple differential equation by Taylor series and Runge- Kutta methods.

(vi) **Numerical integration** : Newton- Cotes formulae, Romberg integration, errors in integration formulae.

(vii) The students should develop computer programs for some of the above numerical methods.

Unit-II

(a) **Running of Advanced scientific Packages** : The students are expected to get hands on experience of running a few selected advanced level scientific software package after a brief introduction to the basic theory and methodology. Ab initio quantum chemical packages such as GAUSSIAN/GAMES with carefully designed exercise for illustrating various features of the packages. Semi- empirical / Dynamic / simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relating drug and catalysis design etc.

(b) **Computer Experiments** : Computer experiments using quantum chemistry – software packages such as GAUSSIAN./GAMESS /MOPAC and modeling software e.g. MM2/AMBER/CHARM etc.

Unit-III

Introduction to networking and Search Using Internet in Chemistry: Development of small computer codes involving simple formula in Chemistry such as Vander Waal's equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy & ionic radii from experimental data. Linear simultaneous equations to solve secular equations with in the Huckel theory, Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge data base. Execution of linear regression, x-y plot, numerical integration & differentiation as well as differential equation solution programmes with data preferably from physical chemistry laboratory.

Unit-IV

(a) **Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock theory.**

Review of the principles of quantum mechanics, Born- Oppenheimer approximation. Slater- Condon rules, hartree- fock equation, koopmans and brillouin theories roothan equation, Gaussian basis sets.

(b) **Configuration Interaction and MC-SCF**
Introduction to CI; Full and truncated CI Theories size consistency introductory treatment of coupled cluster and MC-SCF methods.

Unit-V

(a) **Semi- Empirical theories** : A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on experience on personal computers.

In spotting there should be 5 spots related with instruments, techniques, spectra, safety symbols etc. from the syllabus ; time of spotting is 20 minutes and a separate copy shall be used for the purpose.

Viva Record Total 10 10 150

M.Sc. (FINAL) CHEMISTRY, 2021.

PAPER-V CH-501: SPECTROSCOPY, PHOTO CHEMISTRY AND COMPUTER IN CHEMISTRY

Time : 3 Hours Max. Marks : 75 Unit-1

(a) **Vibrational Spectroscopy** : Symmetry and shapes of AB₂, AB₃, AB₄, AB₅ and AB₆, mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metallo proteins.

(b) **Ultraviolet and Visible spectroscopy** : Various electronic transitions (185-800nm), 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 steric effect in biphenyls.

(c) **Infrared Spectroscopy** : 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, aldehyde, 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, FTIR, IR of gaseous, solids and polymeric materials.

(d) **Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)** : Definition, deduction of absolute configuration, Octant rule for ketones.

(e) **Mossbauer spectroscopy** : Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe⁺² and Fe⁺³ compounds including those of intermediate spin, (2) 12 Sn and Sn⁺⁴ compounds - nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Unit-II

(a) **Nuclear magnetic Resonance spectroscopy** : General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, 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, complex spin-spin interaction between two, three, four and five nuclei (first order spectra,) virtual coupling stereochemistry, hindered rotation, Karplus curve variation of coupling

constant with dihedral angle. Simplification of complex. Fourier transform technique, nuclear overhauser effect (NOE) Resonance of other nuclei-F.P.

(b) **Nuclear Magnetic Resonance of Paramagnetic Substances in**

Solution: The contact and pseudo contact shifts, factors affecting nuclear relaxation, some application including biochemical systems, an overview of NMR of metal nuclides with emphasis on ^{195}Pt and ^{119}Sn NMR.

(c) **Carbon-13 NMR Spectroscopy:** General consideration: chemical shift (aliphatic olefinic, alkyne, aromatic, hetro aromatic acid carbonyl carbon) coupling constants.

Two dimensional NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

(d) **Electron Spin Resonance Spectroscopy:** Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as pH_4F_2 and $[\text{BH}_3]$.

Unit-III

(a) **Photochemical Reactions:** Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(b) **Determination of Reaction Mechanism:** Classification, rate constants and life times of reactive energy state- determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas phase photolysis.

(c) **Photochemistry of Carbonyl compounds:** Intramolecular reactions of carbonyl compounds- saturated, cyclic and acyclic α,β -unsaturated and α,β -unsaturated compounds, Cyclohexadienones.

Intermolecular cycloaddition reactions-determinations and oxetane formation.

(d) **Photochemistry of Alkenes:** Intra molecular reactions of olefinic bond geometrical isomerism, cyclisation reactions, rearrangement 1,4, and 1,5 diens.

Unit-IV

(a) **Photochemistry of Aromatic Compounds:** Isomerisations, additions and substitutions.

(b) **Miscellaneous Photochemical Reactions:** Photo- Fries reactions of anilides. Photo-fries rearrangement.

Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

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

(d) **Organic Solids:** Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

(e) **Mass spectrometry:** Introduction, ion production- EI, CI, FD and FAB factors affecting fragmentations, ion analysis, ion abundance. Mass spectral

(a) **Distribution Functions and Related equation:** Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

(b) **Supercooled and Ionic Liquids:** Super cooled and ionic liquids theories of transport properties: non Arrhenius behaviour of transport properties non Arrhenius behaviour of transport properties cohen trunhball free volume model, configurational entropy model, macedo litovitz hybrid model, glass transition in super cooled liquids.

Book 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, Academmic Press.
- 3- Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
- 4- Introduction to Theroretical Organic Chemistry and Molecular Modeling, W.B. Smith, VCH Weinheim.
- 5- Physical Organic Chemistry, N.S. Lssacs, ELBS/Longman.
- 6- Supramolecular Chemistry, Concepts and Perspective, JM Lehn, VCH.
- 7- The physical Basis of Organic Chemistry, H. Haskill, Oxford University Press.
- 8- An intoductino to Liquied State, P.A. Egelstaff, Academica Press.
- 9- The Dynamic State, A.F.M. barton, Longman.
- 10- Introduction to Statical Themodynamics T.L. Hill Addison Wiley.
- 11- The Liquid State, J.A. Pryde.
- 12- Significant Liquid Structures, H. eyrine and M.S. John

Group-C

CH-508 PAPER :IX-B COMPUTATIONAL CHEMISTRY

Time : 3 Hours

Max. Marks : 75

Unit-I

Fortran / Programming and Numerical Methods: Advanced programming features of FORTRAN /C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

(i) **Solution Equations:** Bisection, regular falsi, Newton- Raphson and related methods for solving polynomial and transcendental equations convergence. Errors and III- conditioning

(ii) **Linear Simultaneous Equations:** Gaussian elimination, gausseidel method gauss-jordan method. Pivoting strategy. Errors and ill conditioning.

(iii) **Eigenvalues and Matrix Diagonalization:** Jacobi and Householder methods, analysis or errors.

scales. Nucleofugacity. The α effect. Ambivalent nucleophiles. Acids base catalysis specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non covalent binding- micellar catalysis.

(c) Steric and Conformational properties : 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.

Unit-III

(a) Radical and Pericyclic Reactivity : Radical stability, polar influences, solvent and steric effect. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions.

Reactivity, specificity and periselectivity in pericyclic reactions.

(b) Supramolecular chemistry : 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 calixarenes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport process. Molecular devices and nanotechnology.

(d) Theory of liquid : Theory of liquids partition function method or model approach single cell models communal energy and entropy. LTD model, significant structure model.

Unit-IV

(a) General properties of Liquids

(i) Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids. Equation of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.

(ii) A classical partial function for liquids, correspondence principle, configuration integral configuration properties.

(b) Methods for Structure Determination and Computational Techniques-

Spectroscopic technique for liquid ceramic structure studies, neutron and X-ray scattering spectroscopy.

Computation techniques - monte carlo and molecular dynamics methods.

Unit-V

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.

Unit-V

Programming in Chemistry : Development of small computer codes involving simple formulae in chemistry, such as Van der Waal equation, PH titration, kinetics, radioactive decay (half life and average life) determination of Normality, Molarity and Molality of Solutions. Evaluation of electronegativity of an atom and lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, Bond angles, dihedral angles etc. of molecules. Extracted use of computer programmes from data base such as Cambridge Data Base.

Use of Computers Programmes : Operations of PC. Data Processing. Running of standard programs and packages such as MS WORD, MS EXCEL-special emphasis on calculations and chart formation. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory. Introduction of working of any one of the packages such as LOTUS/EXCEL/FOXPRO/MOPAC and Word Processing software such as WORDSTAR/MS WORD.

Book Suggested :

- 1- Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- 2- Structural methods in Inorganic Chemistry, E.a.v. Ebsworth, D.W.H. Rankin and S. Craddock, EIBS.
- 3- Infrared and Raman spectra : Inorganic and coordination compounds K Nakamoto Iley.
- 4- Progress in Inorganic chemistry vol., 8, ed., F.A. Cotton, Vol. 15, ed. S.J. Lippard, Wiley.
- 5- Transition Metal Chemistry ed. R.L. Carlin Vol. 3, Dekker.
- 6- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier
- 7- NMR, NQR, EPR and Mossbauer Spectroscopy in inorganic chemistry, R.v. Parksh, Ellis Horwood.
- 8- Practical NMR Spectroscopy, M.L. Martin Heyden.
- 9- Spectrometric identification of Organic Compounds, R.M. Silverstein, G.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.
- 13- Fundamentals of Photochemistry, K.K. Rohtagi- Mukerji, Wiley- Eastern.
- 14- Essentials of Molecular Photochemistry, A. Gilbert and J. baggott, Blackwell Scientific Publication.
- 15- Molecular Photochemistry, N.J. Turro, W.A. Bejamin.
- 16- Introductory Photochemistry, A Cox and T. Camp, Mc- Graw Hill.
- 17- Photochemistry, R.P. Kundall and A. Gillbert, Thomson Nelson.

- 18- Organic Photochemistry, J. Coxon and B. Halton, Cambridge University press.
- 19- Solid State chemistry and its Applications, A.R. West Plenum.
- 20- Principles of the Solid, H.V. Keer, Wiley eastern.
- 21- Solid State Chemistry, N.B. Hannay.
- 22- Solid State Chemistry, D.K. Chakrabarty, New Age International.
- 27- New trends in natural products chemistry-Atta-Ur Rahman and Mi.L. choudhary, Harwood Academic Publishers.
15. Insecticides of Natural Origin Sukhdev, Harwood Academic Publishers.

Group-C**PAPER-IX-A CH- 507 RECENT TRENDS IN PHYSICAL CHEMISTRY****Time : 3 Hours Max. Marks : 75****Unit-I****PAPER-VI CH-502: MODERN TECHNIQUES AND SCOPE OF****CHEMICAL BIOLOGY****Time : 3 Hours****Max. Marks : 75****UNIT-I****(a) Metal Ions in Biological Systems :** Essential and trace metals.**(b) Na⁺/K⁺ Pump** Role of metals ions in biological processes**(c) Bioenergetics and ATP Cycle:** DNA Polymerisation, glucose storage, metal complexes in transmission of energy, chlorophylls photo system I and photo system II in cleavage of water. Model systems.**(d) Transport and Storage of Dioxygen :** Heme proteins and oxygen uptake structure and function of hemoglobin; myoglobin hemocyanins and hemerythrin model synthetic complexes of iron, cobalt and copper.**Unit-II****(a) Electron Transfer in Biology :** Structure and function of metalloproteins in electron transport process – cytochromes and iron-sulphur proteins, synthetic models.**(b) Enzymes :** Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzyme 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 labelling and enzyme modification by site- directed mutagenesis. Enzyme kinetics, Michaelis Menten and lineweaver- burk plots, reversible and irreversible inhibition.**(c) Mechanism of enzyme Action:** Transition – State theory, orientation and steric effect, acid- base catalysis, covalent catalysis, strain or distortion. Example of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.**Unit-III****(a) Kinds of Reactions Catalysed by Enzymes :** Nucleophilic displacement on phosphorus atoms, multiple displacement reactions and the coupling of ATP cleavage to endergonic process. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, b- cleavage and condensation, some isomerization and rearrangement reactions. Enzymes catalyzed carboxylation and decarboxylation.**(b) Co-Enzyme Chemistry :** Co factors as derived from vitamins, coenzymes prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD,**(a) Concept in molecular orbital (MO) and Valence Bond (VB) Theory :**

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 ethane, allyl and butadiene. Qualitative MO theory- ionization 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. Curve- crossing model-nature of activation barrier in chemical reactions.

(b) Principle of Reactivity : Mechanistic significance of entropy, enthalpy and Gibb's free energy, Arrhenius equation. Transition state theory, uses of activation parameters, Hamond's postulate, Bell Evans- Polanyl principles. Potential energy surface model. Marcus theory of electron transfer reactivity and selectivity principles.**(c) Kinetic Isotope Effect :** Theory of isotope effects, primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunnelling effect, solvent effects.**(d) Structural effects on reactivity :** Linear free energy relationships (LFER). The Hammett equation, substituent constant, theories of substituent effects. Interpretation of ρ Values, reaction constant ρ . Deviation from Hammett equation. Dual parameter correlations, inductive substituent constant. The Taft model, σ_1 and σ_p scale.**Unit-II****(a) Solvation and solvent Effects :** Qualitative understanding of solvent solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical index of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scale for specific solvation. Use of solvation scales in mechanistic studies, Solvent effects from the curve crossing model.**(b) Acids, Bases, Electrophiles, Nucleophiles and Catalysis:** Acid base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity

- (b) **Seven- and large membered Heterocycles** : synthesis and reactions of diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocine.
- Unit-III**
- (a) **Five membered heterocycles with one & two heteroatoms** : Synthesis & reactions of Pyrrole, thiophene, furan, pyrazole, imidazole, oxazole and thiazole.
- (b) **Terpenoids and Carotenoids** : Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules : Citral, Geraniol, α -terpineol, Menthol, Zingiberene, Santonin and β -carotene.
- Unit-IV**
- (a) **Alkaloids** : Definition, nomenclature and physiological action, occurrence isolation, general methods of structure elucidation, degradation classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : Ephedrine, (+)-coniine, nicotine, atropine quinine and morphine.
- (b) **Porphyrins** : structure and synthesis of hemoglobin and chlorophyll.
- Unit-V**
- (a) **Steroids** : Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, androsterone, estrone, progesterone, aldosterone. Biosynthesis of steroids.
- (b) **Plant pigment** : Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of quercetin and myrcetin.
- Books Suggested :**
- Heterocyclic chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta springer Verlag.
 - The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
 - Heterocyclic chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
 - Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
 - Contemporary Heterocyclic compounds, R.M. Acheson, John Wiley.
 - An introduction to the Heterocyclic compounds R.M. Acheson, John Wiley.
 - Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Reeds, ed. Pergamon Press.
 - Natural Products : chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborn, Longman Essex.
 - Organic Chemistry, Vol2, I.L. Finar Elbs.
 - Stereoselective synthesis : A practical Approach, M. Nogradi, BCH.
 - Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
 - Chemistry, biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed Kurt Hostettmann, M.P Gupta and A. Marston, Harwood Academic Publishers.
 - Introduction to Flavonoids, B.A. Bohm, Harwood, Academic Publishers.
 - lipic acid, vitamin B12 Mechanisms of reactions catalyzed by the above cofactors.
- (c) **Enzyme Models** : Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, cryptates, cyclodextrins, cyclodextrin based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.
- (d) **Biotechnological Application of Enzymes** : Large-Scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization of 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.
- Unit-IV**
- (a) **Biological cell and its Constituents** : Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.
- (b) **Bioenergetics** : Standards free energy change in biochemical reactions exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP.
- (c) **Statistical Mechanics in Biopolymers** : Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structure. Polypeptide and protein structures, introduction to protein folding problem.
- (d) **Biopolymer interactions** : Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.
- Unit-V**
- (a) **Thermodynamics and Biopolymer Solutions** : Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
- (b) **Cell Membrane and Transport of Ions** : Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport Nerve conduction.
- (c) **Biopolymers and their Molecular Weights** : Evaluation of size, shape, molecular weight and extent of hydration of biopolymers by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.
- (d) **Diffraction Method** : Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy. ORD
- Books Suggested:-**
- Principles of Bioorganic Chemistry S.J. Lippard and J.M. Berg, University Science Books.
 - Bioinorganic chemistry, I Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University science books.
 - Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.

- 4- Progress in Inorganic Chemistry, Vols 19 and 38ed, J.J. Luippard, Wiley.
- 5- Bioorganic chemistry : A Chemical Approach to Enzyme Action, Heeermann Dugas and C. Penny, Springerverlag.
- 6- Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 7- Enzyme Chemistry : Impact and Applications, Ed. Collin J. Sucking Chapman and Hall.
- 8- Fundamental of Enzymology, NC, Price and L. Stevens. Oxford, Universtiy Press.
- 9- Immobilized Enzymes An Introduction and Application in Biotechnology, Michael D. Trevan, John wiley.
- 10- Enzymatic Reaction Mechanisms, C. Waish, W.H. Freeman.
- 11- Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
- 12- Biochemistry : The chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
- 13- Enzyme Mechnisms Ed. M.L. Page and A. Williams, Royal Society of chemistry.
- 14- Principle of Biochemistry, A.L. Lehinger, Worth Publishers.
- 15- Biochemistry . L. Stryer. W.H. Freeman.
- 16- Biochemistry, J. David Rawn, Neil Patterson.
- 17- Biochemistry, Voet and Voet, John wiley.
- 18- Outline of Biochemistry, E.E. Conn and P.K. Stumpt, John Wiley.
- 19- Bioorganic Chemistry : A Chemical Approach to Enzyme Action. H. Dugas and C. Penny, Springer- Verlag.
- 3- Advanced Organic Chemistry reactions mechanisms and structure J marrec John Wiley.
- 4- Principles of Organic Synthesis, RoC Norman and J.M. coxon, blackie academic & Professional.
- 5- Advanced organic chemistry Part-B, F.A. carey and R.J. shutting pleanum press.
- 6- Rodd's chemistry carbon compounds, ed S. coffey, Elsevier.
- 7- Designing organic synthesis S Warren Wiley.
- 8- Organic synthesis – concepts, methods and starting, material J funrhop and G. Penzillin, vertage VCh.
- 9- Some moder methods of organic syntheis W.E. carruthers Cambrid uNiv. Press.
- 10- Modern synthesis reactions, H.Q. house W.A.A. Benjamin.
- 11- Advanced organic chemistry readctions, Mechanisms and structure, March Willy
- 12- Principle of organic synthesis, R h Norman and J.M Cozon, Blackie academic & professional.
- 13- Advanced organic chemistry Part-B.F.A Carey and R.J. Sundberg Plenum press.

Group-B**Paper-VIII-B CH-506 Heterocyclics and Natural Products****Time : 3 Hours Max. Marks : 75****Unit-I**

20- Macromolecules : Structure and Function, F. Woold, Prentice Hall.

(a) **Nomenclature of Heterocycles** : Systematic nomenclature (Hantzsch – Widman system) for monocyclic, fused and bridged heterocyclics.

(b) **Aromatic Heterocycles** : General chemical behaviour of aromatic heterocycles , classifications (Structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in H NMR- spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

(c) **Non aromatic Heterocycles** : strain in bond angle and torsional strain and their consequences in small ring heterocycles.

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

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

(c) **Transition Metal Compounds with Bonds of Hydrogen.**

Unit-II

(a) **Transition Metal δ - Complexes** : Transition Metal δ -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, 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.

(d) **Heterocyclic Synthesis** : Principles of heterocyclic synthesis involving cyclization reaction and cycloaddition reactions with reference to synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Unit-II

(a) **Benzo- Fused Five Membered Hetrocycles** : Synthesis and reactions including medicinal applications of benzopyrroles, benzofuranes and benzothioophenes.

Organometallic Regents : Principles, preparations, properties and applications of the following in organic synthesis with mechanistic details.

(a) **Group I and II Metal organic compounds :** Li, Mg, Hg, Cd, Zn, and Ce compounds

(b) **Transition Metals :** Cu, Pd, Ni, Fe, Co, Rh, Cr, and Ti compounds

Unit-II

(a) **Oxidation :** Introduction, different oxidative processes. Hydrocarbons – Alkenes aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehydes, ketones and carboxylic acids. Amines, hydrazines and sulphides. Oxidations with Ruthenium tetroxide, Iodobenzene diacetate and Thallium (III) nitrate.

(b) **Reduction :** Introduction, different reduction processes. Hydrocarbons- Alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds- aldehydes, ketones, acids and their derivatives, Epoxides. Nitro, Nitroso, Azo and oxime groups. Hydrogenolysis.

(c) **Rearrangements :** General mechanistic considerations – nature of migration, migratory aptitude. Memory, effects. A detailed study of the following rearrangements- Pinacol- pinacolone, Wagner- Meewein, Damjanov, Benzil- Benzilic acid, Favorskii, Arndt- Eistert synthesis, Neber, Beckmann, Hofmann, Curtius Schmidt, Baeyer- Villager, Shapiro reaction. Metallocenes, non Benzenoid aromatics and Polycyclic Aromatics compounds general considerations, synthesis and reactions of some representative compounds.

Unit-III

(a) **Disconnection Approach:** An Introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group- C-X and two group C-X disconnections, chemoselectivity reversal of polarity, cyclisation reactions, amine synthesis.

(b) **Protecting groups :** Principles of protection of alcohol, amine, carbonyl and carboxyl groups.

Unit-IV

(a) **One group C-C disconnections :** Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, uses of acetylenes and aliphatic nitro compounds in organic synthesis.

(b) **Two group C-C disconnections :** Diels – Alder reaction, 1-3 difunctionalised compounds, alpha & beta unsaturated carbonyl compounds, control in carbonyl condensations, 1,5- difunctionalised compounds, Micheal addition and Robinson annulation.

(c) **Ring Synthesis :** Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings aromatic heterocycles in organic synthesis.

Unit-V

Synthesis of Some Complex Molecules : Camphor, Longifoline, cortisone, reserpine, vitamin D, Juvabione, Aphidicolin and Fredericamycin A.

Books Suggested :

- 1- Modern Synthetic Reactions, H.Q. House, W.A. Benjamin.
- 2- Some modern Methods at organic synthesis, W, Carruthers, Cambridge University press.

(b) **Metal in Medicine :** Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

Unit-III

(a) **Homogenous Catalysis:** Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler- Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reactions), oxopalladation reactions, activation of C-H bond.

(b) **Fluxional organometallic compounds:** Fluxionality and dynamic equilibria in compounds such as η^2 -olefin, η^3 - allyl and dienyl complexes

Unit-IV

(a) **Metalloenzymes:** Zn enzymes- Carboxypeptidase and carbonic anhydrase. Iron enzyme catalase, peroxidase and cytochrome P-450. Copper enzyme –superoxide dismutase. Molybdenum oxotransferase enzyme aniline oxidase. Coenzyme vitamin B12.

(b) **Metal storage transport and biomineralisation: Ferritin, Transferrin and siderophores.**

Unit-V

Supramolecular Chemistry : Concepts and language.

(a) **Molecular recognition :** Molecular receptors for different types of molecules including anionic substrates, design and synthesis of coreceptor molecules and multiple recognition.

(b) Supermolecular reactivity and catalysis.

(c) Transport processes and carriage design.

(d) Supramolecular devices supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Books Suggested :

- 1- Principles and application of Organotransition Metal chemistry, J.P. Collaman, L.S Heddus, J.R. Norton and R.G. Finke, 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 Agee International.
- 5- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 6- Bioinorganic Biochemistry, I. Bertini, H.B. Gray, S.J. Valentine, University Science Books.
- 7- Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.
- 8- Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, wiley.
- 9- Supramolecular Chemistry, J.M. Lehn, VCH

Group-A

PAPER : VII B CH-504 METAL COMPLEXES, POLYMERS AND CERAMICS

Time : 3 Hours **Max. Marks : 75**

Unit-I

(a) **Basics of Photochemistry :** Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times. Flash photolysis. Stopped flow technique Energy dissipation by radiative and non-radiative processes. Absorption spectra, Frank-condon principle, photochemical stages- primary and secondary process.

(b) **Properties of Excited States :** Structure, dipole moment, acid- base strengths, reactivity. Photochemical kinetics, calculation of rates of radiative processes. Bimolecular deactivation- quenching.

(c) **Excited states of Metal Complexes:** 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.

Unit-II

(a) **Redox Reaction by Excited Metal complexes :** Energy transfer under condition of weak interaction and strong interaction- exciplex 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 oxidizing character of Ruthenium 2 (bipyridal complex, comparison with Fe (bipy)₃ role of spin orbit coupling life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high energy products, chemical energy into light.

(b) **Metal complex sensitizers :** Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide system, water photolysis, nitrogen fixation and carbon dioxide reduction.

Unit-III

Ceramics Technology :

(a) Description and classification of various minerals based on their chemical compositions, Physical properties and occurrence.

(b) Study in detail of raw materials used in glass, Refractories, White wares, Potteries and Cement

(c) Chemical characteristic of raw materials of alkali and alkaline earth elements, Silica, Silicates, Alumina, Aluminates, Titania, Zirconia and and zircon, Chromatography : Introduction, Paper and thin layer chromatography, Liquid chromatography, Types of liquid chromatography, Column and detection systems. Differential thermal analysis (DTA) and thermo gravimetric analysis (TGA) with suitable examples.

Unit-IV

Polymer technology :

Polymer characterization : polydispersion – average molecular weight concept. Number, weight and viscosity average molecular weights Polydispersity and molecular weight distribution, The practical significance of molecular weight measurement of molecular weights. End-group, viscosity light scattering, osmotic and ultracentrifugation methods, X-ray diffraction

study Microscopy. Thermal analysis and physical testing – tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

Structure and Properties : Morphology and order in crystalline polymers – configurations of polymer chains. Crystal structure 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.

Polymer processing : Plastic elastomers and fibers. Compounding processing techniques calendaring, die casting rotational casting, film casting, injection molding, blow molding, extrusion molding, thermoforming, foaming, reinforcing and fiber spinning.

Unit-V

Commercial Polymers :

Polyethylene, polyvinyl chloride polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers- fire retarding polymers and electrically conducting polymers Biomedical polymers- contact lens. Dental polymers, artificial heart, kidney, skin and blood cells.

Books Suggested :

- 1- Concepts of inorganic photochemistry, A.W. Adamson and P.D. Feischauer, Wiley.
- 2- Inorganic Photochemistry, J. Chem. Educ. Vol. 60, No10, 1983
- 3- Progress in inorganic chemistry, vol 30 ed, s.J. Lippard wiley.
- 4- Coordination Chem. Revs: 1981, vol39, 121, 131; 1975, 15, 321, 1970-97, 113.
- 5- Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti Academic press.
- 6- Elements of inorganic photochemistry, G.J. Willey.
- 7- Textbook of polymer Science, FW Lamba, Prentice Hall
- 8- Physical and Chemistry of polymers, J.M.G. cowie, Biackles Academic and Professional.
- 9- Functional monomers and polymers, K. Takemoto, Y. Inaki and RM Otanbrite.
- 10- Contemporary polymers Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- 11- Polymers of science V.R. Gowariker, N.V. Vuswanathan and J. Sreedhar Wiley- Eastern.

Group-B

Paper :VIII –A CH- 505 ORGANIC SYNTHESIS

Time : 3 Hours

Max. Marks : 75

Unit-I