शहीद नंदकुमार पटेल विश्वविद्यालय, गढ़ उमरिया, ओड़िशा रोड, रायगढ़ SEMESTER SYLLABUS

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SCHEME OF EXAMINATION & DISTRIBUTION OF MARKS

SEMESTER - 1/6

OLINE	3.1 L 1 - 1				
Paper	Title of the Paper (s)	Internal	Term End	Practical	Total
No.	10 s 10 m	Assessment	Exam		Marks
1.	Inorganic Chemistry		·. 80	2000	100
2,	Organic Chemistry, Stereochemistry & Pericyclic Reaction	20:	80		100
3.	Physical Chemistry- I	20	80		100
4.	Spectroscopy And Mathematics/Biology For Chemists	20	80		100
LAB-I	Organic Chemistry				100
LAB-II	Analytical Chemistry	Segara Charles			100
	1.12			TOTAL	600

SEMESTER - II

Paper No.	ীitle of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20.	80		100
2.	Organic Chemistry	20	80		100
3.	Physical Chemistry	20	80		100
4.	Spectroscopy, Diffraction Methods & Computer For Chemists	20	80		100
	Inorganic Chemistry				100
LAB-II	Physical Chemistry		• • • • • • • • • • • • • • • • • • • •		100
				TOTAL	600

SEMESTER - III

Paper	Title of the Paper (s)	Internal	Term End	Practical	Total
No.		Assessment	Exam		Marks
COMP	ULSORY FOR GROUP A, B & C				
1.	Applications Of Spectroscopy	20	80		100
2.	Chemistry Of Bio-Inorganic & Bio-Organic	20	80	:	100
LAB-I	General (Compulsory)			200	200
OPTIO	NAL GROUP-A INORGANIC				
3.	Organotrasition Metal Chemistry	20	80		100
4.	Photo inorganic Chemistry	20	80		100
OPTIO	NAL GROUP-B ORGANIC				
3.	Physical Organic Chemistry	20	80		100
4.	Chemistry Of Heterocyclic Compounds	20	80		100
OPTIO	NAL GROUP-C PHYSICAL				•
3.	Chemistry Of Materials	20	80		100
4.	Advanced Quantum Chemistry	20	80		100
	•	· '		TOTAL	600

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SEMESTER

Paper	Title of the Paper (s)	Internal	Term End	Practical	Total
No.		Assessment	Exam		Marks
COMP	ULSORY FOR GROUP A, B & C			:	2.0
27/21	Photochemistry & Solid State Chemistry	20	80		100
2	Bio Physical & Environmental Chemistry	200.00	80	(4 (b) = 1	100
OPTIO	NAL GROUP-A INORGANIC			- ***	
3.	Bioinorganic Chemistry & Supra- Malecular Chemistry	20	80		100
4.	Agalytical Chemistry	20	80		100
LAB-I	Special			200 -	~ 200
OPTIO	NAL GROUP BORGANIC				
3,33	Medicinal Chemistry	20	80		100
4.	Chemistry Of Natural Product	20	80	201 2 19 January	100
	Soccial	1 13	0 0 40 0 0	200 > .	200
OFTIO	NALI GROUP-C PHYSICAL			2000	A CONTRACT
3	Liquid States:	20	80		100
4	Computation Chemistry	20	80		100
LAB4	Special		The state of the s	200	200
aring.			TOW Secula	TOTAL	600
4			GRAND	TOTAL	2400

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SÉMESTER I PAPER – I INORGANIC CHEMISTRY

UNIT-I

Stereochemistry and Bonding in Main group Compounds – VSEPR theory, Walsh Diagram (Tritland Pentatonic-Molecules) due pur bonds, bent rule and energetic of hybridisation, some simple reaction of covalently bonded, molecules.

UNIT-II

Metal Ligand Bonding – Limitation of Crystal field Theory, Molecular orbital theory, octahedral, Tetrahedral and square planar complexes, π Bonding & molecular orbital theory.

UNIT-III

Electronic spectra of transition metal complexes — Energy levels in an atom, coupling of orbital angular momentum, determination of ground state term, derivation of term symbols. Electronic spectra of Transition metal complexes, Orgel and Tanabe- sugano-diagrams for Transition metal complexes.

UNIT-IV

- Magnetic Properties of transition metal complexes- Anomalous magnetic moment,
 Magnetic Exchange coupling and spin crossover, charge transfer spectra.
- b. Symmetry and Matrix representation- Symmetry Element & Symmetry operation, point Symmetry Group, schoenflies symbols, Matrix Representation of Symmetry Operations, Multiplication Table.

UNIT-V

Group Theory in Chemistry- Definition of group subgroup, relation between orders of a finite group and its sub group. Conjugate relation and classes, reducible & irreducible representations (Representation for Cn. Cnv. Cnh. Dnv. Dnh etc. Groups to be worked out-explicitly)

Books Suggested-

- Group Theory Bhattacharya
- 2. Advance Inorganic Chemistry F.A. Cotton and Wilkinson: John Wiley.
- 3. Inorganic Chemistry J.E. Huhey Harpes & Raw
- 4. Chemistry of the elements N.N. Greenwood & A Earnshow Pergamon.
- Inorganic Electronic Spectroscopy A.B.P. Lever, Elsevier.
- 6. Magneto Chemistry R.L. Carlin Springer Verlag.
- 7. Comprehensive Co-ordination Chemistry, G. Wilkinson R.D. Gillar's and J.A. Mccleverty Pergamon.
- 8. Chemistry Applications of Group Theory F.A. Cotton.

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SEMESTER-I PAPER - II ORGANIC CHEMISTRY, STEREOCHEMISTRY & PERICYCLIC REACTION

UNIT-1

Reaction Intermediates: Generation, structure, stability and reactivity of carbocations, carbanions; free radicals, carbenes, nitrenes, and benzynes. Application of NMR in detection of carbocations.

Nature of Bonding in Organic Molecules: Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrogarbons, Huckel's rule, energy level of I molecular orbitals, annulenes, homoaromaticity, PMO approach.

UNIT-II

Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactitity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral centre, three and erythre isomers, methods of resolution, opticalpurity, enantiotopic and diastereotopic atoms, groups and faces, stereospecfic and stereo selective synthesis. Asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes). Chirality due to helical shape. Stereo chemistry of the compound containing nitrogen, sulphur and phosphorus.

UNITE HE

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate: Potential energy diagrams, transition states and intermediates, methods of determining mechanism, isotope effects. Hammett equation and lipear free energy relationship, substituent and reaction constants.

UNIT-IV

Pericyclic Reactions: Molecular orbital symmetry, frontier orbitals of ethylene 1,3-butadiene, 1,3,5- hexatriene and allyl system. Classification of pericyclic reactions. Wood ward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions, Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antrafacial and suprafacial additions, 4n, 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cyclo additions and cheleotropic reactions. Sigma tropic rearrangements - Suprafacial and antrafacial shifts of H. sigmatropic shifts involving carbon moieties 3,3 and 5,5- Sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.

UNIT-V

Molecular rearrangement: General mechanistic approach to molecular rearrangement reactions, carbocation rearrangement-migratory aptitude and memory effects. Brief study of following rearrangement reactions. Favoroskii, Baeyer-Villigers oxidation, Stork enamine reaction, Shapiro reaction, Sommelet rearrangement, wittig's rearrangement, Grovenstein-Zimmerman rearrangement.

Books Suggested:

1. Advanced Organic Chemistry - Reaction Mechanism and Structure, Jerry March, John Wiley.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

- 2. Advanced Organic Chemistry F.A. Carey and R.K. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry- Peter Syke longman.
- 4. Structure and Mechanism in organic chemistry C.K. Ingold, Cornell University Press.
- 5. Organic Chemistry R.T. Morrison and R.N. Boyed Prentice Hall.
- 6. Modern Organic Reactions H.O. House, Benzamic.
- 7. Principles of Organic Synthesis R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional:
- 8. Pericyclic Reaction S.M. Mukherji.
- 9. Reaction Mechanism in Organic Chemistry S.M. Mukherji and S.P. Singh Macmilan,
- 10. Stereochmistry of Organic compounds D. Nasipuri New age International.
- 11. Sterochemistry of Organic Compounds P.S. Kalsi, New Age International.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-1 PAPER - III PHYSICAL CHEMISTRY-1

UNIT- I Quantum Chemistry:

Introduction in Exact Quantum Mechanical Result: The Schrödinger equation and the postulates of quantum mechanics. Discussion of solution of the Schrödinger equation to some model systems, viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate methods: The various theorems, linear variation principle. Perturbation theory (first order and non – degenerate). Application of variation method and perturbation theory to the Helium atom.

Angular Momentum: Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Eigenvalue of angular momentum, operator using ladder operators, addition of angular momenta, spin anti-symmetry and Pauli Exclusion Principle.

UNIT-11 Atomic Chemistry:

Electronic Structure of Atoms: Electronic configuration, Russell – Saunders term and coupling scheme. Slater – Condon parameters, term separation energies of pⁿ configuration, term separation energies for dⁿ configurations, magnetic effects: spin – orbital coupling and Zeeman splitting, introduction to the method of self- consistent field, the virial theorem.

Molecular Orbital Theory: Huckel theory conjugated system, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. introduction to extended Huckel theory.

UNIT-III Chemical Dynamics:

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Amherius 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 nuclear magnetic resonance method, Dynamics of melecular 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:

Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Calvin equation), and Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film on liquids (Electro-Kinetic phenomenon), catalytic activity of surfaces.

Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ions binding to micelles, thermodynamics of micellization — phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

UNIT- V

Macromolecules: Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetic of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination(osmometry, viscometry, diffusion and light scattering method), sedimentation, chain configuration of macro molecules, calculation of various chain structures:

Books Suggested:

- 1. Physical Chemistry; P. W. Atkins, ELBS.
- 2, introduction to Quantum Chemistry; A. K. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry; Ira. N. Levine, Prentice Hall.
- 4. Coulson's Valence, R. Mc Weeny, ELBS.
- 5. Micelles Theoretical and Applied Aspects; V. Moroi, Plenum.
- Introduction to Polymer Science; V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar, Wiley Eastern.
- 7. Physical Chemistry of Surface: A. W. Anderson and A. Gast, Wiley.
- 8. Surfaces, G. Attard and C.Barnes, Oxford Univ. press.
- 9. Introduction to Solid state physics. Kittel, Wiley.
- 10. Crystal structure determination; W. Clegg, Oxford University Press.

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SEMESTER I PAPER - IV SPECTROSCOPY AND MATHMATICS/BIOLOGY FOR CHEMISTS SECTION- A

UNIT-1

spectroscopy

Unifying Principles: Electromagnetic radiation, Interaction of Electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and Natural line width and natural line broadening. Transition Probability, results of the time dependent perturbation theory, transition moment. Selection rules, intensity of spectral lines. Born-Oppenheimer approximation, Rotational, Vibrational and Electronic Energy Levels.

UNIT- II

Microwave Spectroscopy: Classification of Molecules, rigid rotor model effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, Nuclear and Electron spin Interaction.

Raman Spectroscopy: Classical & Quantum Theories of Raman Effect, Pure rotational, vibrational & vibrational rotational Raman Spectra, Selection rules, Metual exclusion Principle, Resonance Raman Spectroscopy, Coherent, Antistokes, Raman Spectroscopy (CARS). Allegan allegan

UNIT- III

Vibrational Spectroscopy: Infrared Spectroscopy - Review of linear harmonic oscillator, vibrational energies of diatomic molecules, Zero point energy, force constant and bond strengths annormonicity, morse potential energy diagram, vibrational, rotation spectroscopy. P.Q.R. branches. Breakdown of oppenheimer approximation. Vibration of poly atomic molecules. Selection rules, normal modes of vibration, group frequencies overtones hot bands factors affecting the band positions and intensities for IR region.

SECTION- B **MATHEMATICS FOR CHEMISTS** (For Students without Mathematics in B.Sc.)

UNIT- IV

Vector and Matrix Algebra

Vectors: - Vector dot, cross and triple products etc. The gradient divergence and curl. Vector calculus, gauss Theorem divergence Theorem etc.

Matrix Algebra: - Addition and Multiplication, Inverse, adjoint and transpose of matrices. Special matrices. (Symmetric, Skew symmetric, diagonal, unitary etc.) And their properties, matrix equation, Homogeneous, Non Homogeneous linear equations.

Differential Calculus: Functions, continuity and differentiability rules for differentiation, Applications of differential calculus, including maxima and minima. Exact & Inexact differentials with their Application to thermodynamics properties. Integral calculus, basic Rules for Integration, Integration by parts, partial fraction and substitution. Reduction formulae, Applications of integral calculus. Functions of several variables.

UNIT- V

differential equations: Variables-Separable and Exact First-order, differential equation, homogeneous, Exact and linear equation. Applications to Chemical Kinetics, Secular Equilibrium quantum chemistry.

Permutation and Probability: Permutations and combinations, probability and probability theorem, probability curves, average, root mean square and most probable errors, examples from kinetic theory of gases.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

OR SECTION- B BIOLOGY FOR CHEMISTS (For Student without Biology In B.Sc.)

UNIT- IV

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells intercellular organistics and their functions. Comparison of Plant and animal cells: Overview of metabolic processes- catabolism and anabolism. ATP: The biological Energy currency. Origin of life - unique properties of carbon, Chemical evolution and rise of living systems. Introduction to bio molecules, building blocks of Bio-macromolecules.

Carbohydrates: Conformation of mone-saccharides, structure and function of important derivatives of mone-saccharide. Like glycosides deexy sugar myoingstol, Aminosugar, disaccharides and polysaccharides structural. Poly saccharides cellulose and chitin. Storage polysaccharides starch and glycogen. Carbohydrate of glycospicitin and glycolipids. Rele of sugar in biological recognition. Blood group substances: Ascorbic Acid, Carbohydrate metabolism, Krebs cycle, Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, pentose phosphate pathway.

UNIT- V

Lipids: Fatty acids, essential fatty acids, structure and function of triglycerals glycerophospholipids, Sphingolipids cholesterol, bile acids, presta-glandins lipoprofeins-composition and function role in atherosclerosis. Properties of lipid aggregates micelles bilayers: Liposomes and their possible biological functions, Biological membranes, fluid mesaic model of membrane spectra liquid metabolism. β-Oxidation, of fatty acids.

Amino acids, Peptides and Proteins: Chemical & enzymatic hydrolysis of proteins to peptides, Amino Acid sequencing, secondary structure of proteins, forces responsible for holding of secondary structure, or helix, B-sheets super secondary structure, triple helix structure of collagen, Tertiary structure of protein folding and domain structure. Quaternarystructure. Amino Acid metabolism, degradation and biosynthesis of Amino acid. Sequence determination. Chemistry of Oxytocin and tryptophane releasing hormones (TRH)

Nucleic Acid: Purine, Pyrimidine, bases of Nucleic acid, base pairing, via H-bonding, structure of Ribo Nucleic Acid (RNA) & D.N.A. deoxy ribonucleic acid, double helix model of DNA and forces responsible for holding at chemical and Enzymatic Hydrolysis of Nucleic Acid. The Chemical bases of heredity, an overview of replication of DNA. Transcription, translation and genetic code, chemical synthesis of mono and Trinucleosides.

Book Suggested for Spectroscopy:

- 1. Modern Spectroscopy J.M. Hollas Hohnwiley.
- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey Interscience.
- 3. NMR, NQR, ESR and mossbaure spectroscopy in Inorganic chemistry :- R.V. Parish, Ellis Harwood.
- 4. Physical Method in Chemistry R.S. Drago, Saunders College.
- 5. Introduction to Molecular Spectroscopy G.M. Barrow, Mcgraw Hill.
- 6. Basic Principle of Spectroscopy- R. Chang Mcgraw Hill.
- 7. Theory and Application of Uv Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
- 8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

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- 9. Introduction to magnetic Resonance A. Carrington and A.D. Maclachalan Harper & Row. or of earl
- H. Kaur, Spectroscopy, Wiley

Books: Mathematics for chemists:

- The Chemistry Mathematics Book: E.Steiner, Oxford University Press.
- 2. Mathamatics for Chemistry Doggett and Sectcliffe longman.
- 3. Mathematical preparation for physical chamistry—F. Daniels Mcgrow Hiti.
- 4. Chemical Mathematics D.M. Hirsl-Longmann.
- 5. Applied Mathematics for Physical Chemistry LR. Barrate, Prentice Hall.
- Basic Mathematics for Chemists Tebbutt Wiley.

Books -Biology for chemists

- Principles of Biochemistry: A. L. Lehninger, Worth Publishers.
- 2. Biochemistry, L. Stryer, We H. Freeman.
- 3. Biochemistry, J. David Rawn, Neil Patterson
- 4. Biochemistry, Voet & Voet John Wiley.
 5. Biochemistry, Jain & Jain S. Chang.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER I LABORATORY COURSE - I ORGANIC CHEMISTRY

1. Qualitative Analysis:-

Separation, Purification and Identification of compounds of Binary Mixture, T.L.C. and Column chromatography. I.R. Spectra may be used for functional group identification of compound by suitable derivatives preparation and determination of their melting points.

- 2. Organic Synthesis:-
 - 1. Bromination Prepration of p-Bromo Aniline from Acetanilide.
 - 2. Nitration Prepration of p-Nitro Aniline from Acetanilide
 - 3. Hoffman Bromide Reaction, Prepration of Anthranilic Acid from Pthallic anhydride.
 - 4. Aldol Condensation Dibenzal acetone from Bazaldelyde.
 - 5. Sandmeyer Reaction -
 - o-Chloro Benzoic Acid from Anthranilic Acid.
 - p- Chloro toluene from Toludine.
 - 6. Friedal Craft Reaction 🛘 -Benzoyl.Propionic Acid from Succinic Anhydride and Benzene.
 - 7. Oxidation Adipic Acid by Chromic Acid oxidation of cyclohexanol.
 - 7. Diazotization:-
 - Preparation of methyl orange from Sulphanilic Acid.
 - Phenyl Azo- □. Naphthol from Aniline.
 - 8. Preparation of Acridone from N- Phenyl anthranilic acid.
 - 9. Grignard's reaction: Synthesis of tripheny Imethanol from Benzoic acid.

Note: Two stage preparation. Preparation of pure and crystalline compound based on any two of above principals with conformation of melting point.

3. Quantitative Analysis:-

2.

- 1. Determination of the percentage or number of Hydroxyl group in an organic compound by Acetylation method.
- 2. Estimation of Amines/Phenols using Bromate Bromide Solution / or Acetylation method.
- 3. Determination of equivalent- weight of carboxylic compound.
- 4. Estimation of carboxyl group by tritration / silver salt-method.
- 5. Estimation of Carbonyl group by Hydrazone method.
- 6. Estimation of Glycine by titration.

Instruction to Practical Examiners in Chemistry Semester -I

 The Board of Examiners; one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations

S. No.	Lab. Course (branch)	Max. Marks	Duration		
1.	I- Organic Chemistry	100	5 hrs.		
2.	II- Analytical Chemistry	100	5 hrs.		
The distribution	n of marks is as under. Marks of Ex	c-students are given in	parentheses.		
a) Qualitative Analysis of mixture containing two Organic compounds 30 (40) marks					

(a) Qualitative Analysis of mixture containing two Organic compounds 30 (40) marks (b) Preparation 10 (15) marks

(c) Estimation 20 (25) marks
(d) Viva voice 20 (20) marks
(c) Sessional 20 (-) marks

Total-100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER I LABORATORY COURSE II ANALYTICAL CHEMISTRY SECTION- A

INSTRUMENTATION AND COMPUTERS

1. Error Analysis & Statistical data Analysis:-

Errors, types of errors, Minimization of Error, Statistical treatment for error analysis, standard deviation, Relative standard deviation, Linear least square. Calibration of volumetric apparatus burrettes pipette, standard flask, weight box etc.

2. Volumetric Analysis:-

Basic Principles, determination of I₂ and saponification values of oil sample determination of DO, COD, BOD, Hardness of water samples.

3. Chromatography:-

Separation of Cations and anions by (A) Paper Chromatography, (B) Column Chromatography.

SECTION-B

4. pH Metry / Potentiometry / Conductometry fitration :- ... Determination of strength of acid etc.

5. Flame Photometry / AAS/FIA/Colorimetry :--

Determination of Cations / anions and metal tons eg. Na⁺, K⁺, Ca²⁺,SO4²⁻NO₂, Fe, Mo, Ni ,Cu, Zn etc.

6. Spectro Photometry :-

Verification of Beer - Lambert Law. Molar Absorptivity calculation, Plotting graph to obtain I max etc. effect of pH in aqueous coloured system. Determination of metal ions eg. Fe, Cu, Zn, Pb etc

7. Nephelometry / Turbidimetry :- Determination of chlorine, sulphate phosphate turbidity

etc.

8. Application of Computer in Chemistry:- As Specified in Theory paper in section if (A).

For Lab. Course -II (Analytical Chemistry):

(a)Two practical exercise (one from each section)
(at least one of these will be based on instrumental analysis)
(b) Viva voice
(c) Sessional

60 (80) marks
20 (20) marks
20 (-) marks

Total- 100 (100) marks
As far as possible all the exercises as laid down in the syllabus are set. The scale of
marking will be determined by examiners in accordance with the nature of exercises.
Sessional marks will be awarded by External Examiner in consultation with the internal
Examiner

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SEMESTER-II PAPER -I INORGANIC CHEMISTRY

Note: - Two questions will be asked from each Unit and student will have the choice to attempt any one question from each unit.

Unit-1

metal ligand Equilibrium in solution: - Step wise & overall formation constants and their interaction, trends in step wise formation constants, factors affecting the stability of Metal Complexes with reference to nature of metal ion and ligand.

Unit- 2

Reaction mechanism of transition metal complexes: Energy profile of a reaction, reactivity of metal complexes, Inert and Labile complexes. Kinetic application of valence bond & crystal field theories. Kinetics of octahedral substitution acid hydrolysis, factors affecting acid hydrolysis. Base hydrolysis, Anation reactions Reactions without metal ligand bond cleavage, substitution reactions in square planar complexes. The trans effect.

Unit-3

Metal Complexes:

- (A) Mechanism of the substitution reaction, Redex reactions, Electron transfer reactions, mechanism of one electron transfer reaction.
- (B) Metal Clusters- **Higher** boranes , carboranes, metalloboranes and metallocarboranes, Metal carbonyl.

Unit-4

- (A) Metal Carbonyls, Structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls.
- (B) Nitrosyl :- Preparation, bonding, structure & important reactions of transition metal nitrosyl, dinitrogen complexes, tertiary phosphine as ligand.

Unit-5

Isopoly and Heteropoly Acid & salt: Isopoly acids of transition metals Mo, W,V, Nb, Ta.

Heteropoly acids and salt of Mo, W, Structure of heteropoly acids

Books Suggested:-

- 1. Advanced Inorganic chemistry: F.A. Cotton and Wilkinson: John Wiley.
- 2. Inorganic Chemistry : J.E. Huhey, Harpes & Row
- 3. Chemistry of the elements: N. N. Greenwood & A Earnshow Pergamon.
- 4. Inorganic Electronic Spectroscopy A. B.P. Lever, Elsevier
- 5. Magnetochemistry R.L. Carlin, Springer Verlag.
- Comprehensive Co-ordination Chémistry G. Wilkinson, R.D. Gillars and J.A. McCleverty Pergamon.
- 7. Chemistry Applications of Group Theory F.A. Cotton.
- 1. Group Theory: Bhattacharya.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-II PAPER - II ORGANIC CHEMISTRY (REACTION MECHANISM)

UNIT-1

Electrophilic substitution reactions:-

"Aliphatic" electrophilic substitution: - Biomoleculear mechanism: SE² SE1 and SE_i mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Gattermann Koch reaction, vilsmeir reaction.

UNIT-II

Nucleophilic Substitution reactions:-

Aliphatic nucleophilic substitution: The $S_N 2$, $S_N 1$, mixed $S_N 1$ and $S_N 2$ and $S_N 3$ and

Aromatic Nucleophilic substitution: The S_NAr, S_N¹, benzyne and S_{RN}¹ mechanisms, Reactivity-effect of substrate structure. Leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT- III

Free Radical reactions

Types of free radical reactions, Free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridge head. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), exidation 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.

DIMIT: IV

(a) Addition to Carbon-Carbon Multiple Bonds

Contract Contract Con-

Mechanism and stereo chemical 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. Hydroborations Michael reaction, epoxidation.

(b) Addition to Carbon-Hetero Multiple bonds :

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters nitriles. Addition of Grignerd's reagents, organization and organishium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enclates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Hydrolysis of ester and amides, Ammonolysis of esters.

UNIT-V

Elimination reactions:

The E_2 , E_3 and E_{10B} mechanism and their spectrum, orientation of double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

Books Suggested,

- 1. Advanced Organic Chemistry Reaction Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry F.A. Carey and R.K. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry Peter Sykes-longman.
- 4. Structure and Mechanism in organic chemistry. C.K. Ingold, Cornell University Press.
- 5. Organic Chemistry R.T. Morrison and R.N. Boyed; Prentice Hall.
- 6. Modern Organic Reactions H.O. House, Benzamic.
- 7. Principles of Organic Synthesis R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional.
- 8. Reaction Mechanism in Organic Chemistry S,M. Mukherji and S.P. Singh Macmillan

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-II PAPER -III PHYSICAL CHEMISTRY KINETICS & ENERGETICS

UNIT-1

THERMODYNAMICS: Classical Thermodynamics: Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non- ideal systems: Excess functions for non-ideal solutions. Activity, Activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule to three component systems, second order phase transitions.

UNIT- II

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions—translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function, application of partition function. Heat capacity behavior of solids - chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

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

UNIT-III

ELECTROCHEMISTRY: Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions, Debye-Huckel Jerum mode. Thermodynamics of electrified interface equations, derivations of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stem, Graham-Devanthan - Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, Quantum aspects of charge transfer at electrodes- solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces - theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light a semi-conductor solution interfaces.

UNIT- IV

Electro-catalysis - influence of various parameters, Hydrogen electrode. Bioelectrochemistry, threshold membrane phenomena, Nernst-Plank equation, Hodges-Huxley equation, core conductor models, electrocardiograph. Polarography theory, Ilkovic equation, half wave potential and its significance, Introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

UNIT- V

(a) 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 surface.

(b) NEUTRON DIFFERACTION-

Scattering of neutron by solid and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

Book Suggested

- 1. Physical Chemistry P.W. Atkins, ELBS
- 2. Introduction to Quantum Chemistry A.K. Chandra, Tata McGraw Hill
- 3. Quantum Chemistry Ira N. Levine, Prentice Hall-
- 4. Coulson's Valence R. McWeeny, ELBS
- 5. Chemical Kientics K.J. Laidler, McGraw Hill
- 6. Kinetics and mechanism of chemical transformation J.Rajaraman and J.Kuriacose;
- 7. Micelles, Theoretical and Applied Aspects V. Moroi, Plenum.
- 8. Modern Electrochemistry Vol.1 and II J.O.M. Bockris and A.K.N.Reddy, Plenum.

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9. Introduction of Polymer Science - V.R.Gowarikar, N.V.Vishwanathan and J.Sridhar Wiley Easter

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M.Sc. CHEMISTRY SEMESTER-II

PAPER -IV SPECTROSCOPY, DIFFRACTION METHODS & COMPUTER FOR CHEMISTS

UNIT- Î

Electronic Spectroscopy:-

A. Atomic Spectroscopy: - Energy of Atomic orbitals: Vector Representation of momenta & vector coupling, spectra of Hydrogen atom, alkali metal, atoms

B. Molecular Spectroscopy: - Energy levels; Molecular orbitals, vibration, transition, vibrational progression and geometry of the excited states, Franck-Condon principle. Electronic spectra of polyatomic, molecules, Emission Spectra.

C. Photo Electronic Spectroscopy - Basic principles. Photo-electic effect Ionisation process. Photo Electron Spectra of simple molecules, E.S.Ca), Chemical Information of E.S.C.A., Auger Electron Spectroscopy-basic-idea.

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UNIT-II

all the second of the second Magnetic Resonance Spectroscopy:

A). Nuclear Magnetic Resonance Spectroscopy :- Nuclear Spin, Nuclear resenance, saturation, shielding of magnetic nuclei chemical shift and its measurements factors influencing chemical shift deshielding splinspinshieraction. Fastors influencing coupling constant "J", classification (ABX, AMX, ABC, A,B, etc),

spin decoupling basic ideas about instruments.

B. Electron Spin Resonance Spectroscopy: - Basic principle, Zero field splitting and orbital energy degeneracy, factors affecting the 'g' value, isotopic and anisotopic hyperfine coupling constant. Spin densities and Applications of ESR

C. Nuclear Quadrupole Resonance Spectroscopy quadrupole nuclear, quadrupole

moment electric field gradients, coupling constant splittings. Applications

D. Photoacoustic Spectroscopy :- Basic principle of photoacoustic spectroscopy (PAS), PAS gases and condensed systems, chemical & surface application.

UNIT- III

X-ray Diffraction:-

Bragg's condition. Miller indices, Laue-method, Bragg's method, Debye-scherrer method of X-ray structural analysis of crystals. Index- Reflections identification of unit cell 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.

UNIT- IV

Introduction to Computer and Computer Programming in "C"

Computer Fundamental; - Introduction to Computer organisation. Operating System, DOS, Introduction to UNIX and Window. Computer Languages Principle of programming Algorithm and flow charts.

Programming in C:- Structure of a C Programming, constants, variables, operators and Expressions, data Input & output, decision making, branching and looping statements arrays, well defined functions pointes structure and unions, Format statement. Termination statements. Branching statements such as IF of GO TO statement, LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION, DO statement. FUNCTION and SUBROUTINE, COMMON and DATA statements.

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M.Sc. CHEMISTRY

UNIT- V

Programming in Chemistry and use of Computer Programmes.

- 1. Development of small computer codes Involving simple formulae in Chemistry such as Vander waats Equation, pH Titrations, Kinetic. Radioactive Decays. Evaluation of Lattice Energy and Ionic radie secular equation (within Huckel Theory), Elementry, structural features, such as, bond lenths, bond Angle, dihedral angles etc. Of molecules extracted from a database.
- Introduction and use of computer package MS-Word and Excel. Preparation of graphs and Charts.

Book Suggested for Spectroscopy

- 1. Modern Spectroscopy J.M. Hollas Hohnwilev.
- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey interscience.
- 3. NMR, NQR, ESR and mossbaure spectroscopy in Inorganic chemistry: R.V. Parish, Ellis Harwood.
- 4. Physical Method in Chemistry R.S. Drago, Saunders College,
- 5. Introduction to Molecular Spectroscopy G.M. Barrow, Mcgraw Hill.
- 6. Basic Principle of Spectroscopy- R. Chang Mcgraw Hill.
- 7. Theory and Application of UV Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford
- 8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.
- Introduction to magnetic Resonance. A. Carrington and A.D. Maclachalan Harper & Row.
- Spectroscopy by Kalsi

Books suggested for Computers

- 1. Computer and Common Sense: R. Hunt and J. Shelley Prentice Hall.
- 2. Computational Chemistry A.C. Norris,
- 3. Micro Computer Quantam Mechaniscs, J.P. Kilingbeck, Adam Hilger,
- 4. Computer Programming in fortran IV V. Rajaraman, Prentice Hall.
- 5. An Introduction to Digital Computer Design, V.Rajaraman and T. Radha Krishanan Prentice Hall.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-II LABORATORY – COURSE I INORGANIC CHEMISTRY

Note- Students is accepted to complete all exercises.

 Qualitative analysis of mixture containing eight radical including some less common metal ions among the following by common method (Preferably semi-micro method)

Group-A

Basic Radicals : - {Ag, Pb, Hg, Cu, Cd, Bi, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, co, Ni, Ba, Sr, Ca, Mg, Na, K, NH, }

Acid Radicals: - $\{CO_3, SO_4, SO_3, NO_3, F, Cl, Br, I, NO_2, BO_3, C_2O_4, PO_4\}$

Group-B

Basic Radicals: - {Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.}

Acid Radicals: -{SiO4, Thiosulphate, Ferrocynide, Ferricyanide, Chromate, Arsenite,

Arsenate, Permanganate }

Note - The mixture to be analysed by the students must contain at least one basic and one acid radical from Group B.

2. Quantitative Analysis:-

Involving two of the following in ores, alloys or mixture in solution- one by volumetric and other by gravintetric method Ag, Cu, Fe, Cr, Mn, Ni, Zn, Ca, Mg, Chloride, Sulphate.

3. Estimation of:-

(A) Phosphoric acid in Commercial ortho phosphoric acid.

(B) Borle Acid in Borax.

- (C) Ammonium Ion in Ammonium Salt,
- (D) MnO2 in pyrolusite
- (E) Available Chlorine in bleaching powder.
- (F) H₂O₂ in commercial sample.

Students are expected to perform at least three exercises From above during laboratory work.

- Preparation of selected Inorganic compounds and study of their properties by various method, including IR; Electronic Spectra, Mossbaur, ESR. Spectra+ Magnetic susceptibility etc.
 - (i) V0 (acac)₂
 - (ii) cis K [Cr(C₂O₄)₂(H₂O)₂] ,
 - (iii) [Co(NH₃)₆]Cl₃

trans $K[Cr(C_2O_4)_2(H_2O)_2]$,.2 H_2O

- (iv) Na (Cr (NH₃)₂ (SCN)₄)
- (v) Mn (acac)3
- (vi) $K_3[Fe(C_2O_4)_3]$
- (vii) Prussian Blue Turnbull's Blue....
- $(viii) [Co(NH_3)_6] [Co(NO_2)_6]$
- (ix) Hg [Co (SCN)4]
- (x) $[Ni(NH_3)_4]CI_2, [Ni(NH_3)_4]CI_2$
- (xi) Ni (DMG) $_2$ (xii)[Cu(NH $_3$) $_4$]SO $_4$
- (xii) K₃[Cr(C₂O₄)₃].3H₂O
- (xiii) [Cu(NH₃)₄]SO₄

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-II LABORATORY COURSE- II PHYSICAL CHEMISTRY

1. Adsorption:-

- a. Verification of Freundlich's Adsorption Isotherm.
- b. To study surface tension concentration relationship for solutions (Gibbs equation).

2. Phase Equilibria:

- a. Determination of congruent composition and temperature of binary system e.g. diphenylamine – benzophenone system.
- b. Determination of glass transition temperature of given salt e. g. CaCl₂ conductometrically.
- To construct the phase diagram for three component system e. g. chloroform, acetic acid and water.

3. Chemical Kinetics

- a. Hydrolysis of an ester/ionic reactions.
- b. Determination of the velocity constant of hydrolysis of an ester. Determination of effect of (a)change of temperatures, (b)change of concentration of reactants and catalyst and(c)ionic strength of the media on the velocity constant of media.
- c. Determination of the rate constant for the oxidation of iedide ions by hydrogen peroxide
- d. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ions oxidized by persulphate ion).

4. Conductometry

- a. Determination of solubility of sparingly soluble salt (eg, PbSO₄, BaSO₄)
 Conductometrically.
- b. Determination of the strength of strong and weak acids in a given mixture conductometrically.
- c. Determination of dissociation constant of weak electrolyte by conductometer.
- d. Determination of velocity constant, Order of reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide.

5. pH Metry/Potentiometry

- a. Determination of the strength of strong and weak acid in a given mixture using pH meter/potentiometer.
- b. Determination of dissociation constant of weak acid by pH meter.
- c. Determination of concentration of acid in given buffer solution by pH meter.
- d. Determination of strength of halides in a mixture potentiometrically.
- e. Determination of the valency of mercurous ions potentiometrically.
- f. Determination of the strength of strong acid, weak acids in a given mixture using a potentiometer/ pH meter.
- g. Determination of temperature dependence of EMF of a cell.
- b. Determination of the formation constant of silver- ammonia complex and stoichiometry of the complex potentiometrically.
- i. Determination of activity and activity coefficient of electrolytes.
- j. Determination of thermodynamic constant. $\Delta G_1\Delta S$ and ΔH for the reaction by e.m.f. method. $Z_1 + H_2SO_4 = Z_1SO_4 + H_2$
- k. Determination of the dissociation constant of monobasic / dibasic acid

6. Polarimetry:-

Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter. Enzyme kinetic – inversion of sucrose.

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M.Sc. CHEMISTRY

7. Solutions:

a. Determination of molecular weight of non-volatile and non- electrolyte/electrolytes by cryoscopy method and to determine the activity coefficient of an electrolyte.

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

Instructions to Practical Examiners in Chemistry.

 The Board of Examiners - one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations.

S.No.	Branch	Marks	Duration
(i). Lab Cours	se-I Inorganic Chemistry	100	10 hours
(ii) Lab Cour	se-II Physical Chemistry	100	05 hours

- 2. Sessional marks will be awarded by External Examiner in consultation with the Internal Examiner.
- 3. The distribution of marks is as under. Marks for Ex-students are given in parentheses.

For Lab. Course -I (Inorganic Chemistry):

- Qualitative analysis of mixture containing not more than 8 radicals by semi-microMethod only.

 32 (42) marks
- Quantitative analysis (involving separation) of a solution containing 2 metals, one of these is to be estimated gray/metrically and the other volumetrically.

• S = - S - 3	18 (23) marks
c. (c) Preparation	10 (15) marks
d. (d) Viva voce and manipulation	20 (20) marks
e. (e) Sessional	20 () marks
	Total 100 (100) marks

For Lab. Course -II (Physical Chemistry):

(a) One practical exercise	
	60 (80) marks
(b) Viva voice and manipulation	20 (20) marks
(c) Sessional	20 (-) marks

Total 100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER III COMPULSORY FOR GROUP A, B & C PAPER- I APPLICATIONS OF SPECTROSCOPY

UNIT-1 INORGANIC CHEMISTRY

Vibrational Spectroscopy: Symmetry and shape of AB₂, AB₃, AB₄, AB₅, AB₆ mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly metallo-proteins:

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.

Nuclear Magnetic Resonance of Paramagnetic substances in solution: Factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides with emphasis ¹⁹⁵Pt and ¹¹⁹Sn NMR.

UNIT- II ORGANIC CHEMISTRY

Ultraviolet and Visible Spectroscopy: Instrumentation and sample handling various electronic transition (185-800 nm) Beers-Lambert law, effect of solvent on electronic transitions, ultra-violet bands for carbonyl compounds, dienes, conjugated Polyenes, Fieser-Woodward rule for conjugated dienes and carbonyl compounds, ultra-violet spectra of aromatic and Heterocyclic compounds, steric effect in biphenyls.

Infra-Red Spectroscopy: Instrumentation and Sample Handing characteristic, vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohol, ethers, phenols and amines. Detailed study of Vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, Lactams and conjugated carbonyl compounds), Effect of Hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance FT IR. IR of gaseous, solids and polymeric materials

UNIT-III

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, chemical shift, spin-spin interaction, Shielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, mercaptol) complex, spin-spin interaction between two, three, four and five nuclei (first order spectra) vicinal coupling, stereochemistry, Hindered rotation, Karplus curve, variation of coupling constant with dihedral angle. Solvent effect, Fourier Transform Technique, Nuclear overhouser effect (NOE).

UNIT-IV

Carbon-13 NMR Spectroscopy- General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, Heteroaromatic and carbonyl carbon) coupling constants.

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) - Definition, deduction of absolute configuration, octant rule for ketone.

UNIT-V

Mass Spectrometry- Introduction, ion production-EL, CL, F.D Factors affecting fragmentation, ion analysis. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, Nitrogen rule, Examples of mass special fragmentation of organic compounds with respect to their structure determination.

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Books Suggested-

- 1. Modern Spectroscopy- J.M. Hollas Hohnwiley.
- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey interscience.
- 3. NMR, NQR, ESR and Mossbaure spectroscopy in Inorganic chemistry- R.V. Parish, Ellis Harwood. 4. Physical Method in Chemistry – R.S. Drago, Saunders College.
- 5. Introduction to Molecular Spectroscopy G.M. Barrow, Mcgraw Hill.
- 6. Basic Principle of Spectroscopy R. Chang Mcgraw Hill.
- 7. Theory and Application of UV Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
- 8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.
- 9. Introduction to magnetic Resonance, A. Carrington and A.D. Maclachalan Harper &
- 10. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Raniin and Cradock, ELBS.
- 11. Progress in Inorganic Chemistry, Vol. 8 Ed. F.A. Cotton Vol. 15 Ed. S.J. Lippard Wilev.

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SEMESTER III COMPULSORY FOR GROUP A, B, C PAPER- II

CHEMISTRY OF BIO-INORGANIC & BIO-ORGANIC

UNIT- I BIO-INORGANIC CHEMISTRY:

Metal lons in Biological Systems- Essential and trace metals.: Na+IK+ pumps- Role of metal ions in biological processes. Bio-energetic and ATR cyclo: DNA polymerization, glucose storage; metal complexes in transmission of energy, chlorophylls, Photosystem-land Photosystem-II in Cleavage of water, Model systems.

UNIT-II

Transport and Storage of Dioxygen- Heme protein and oxygen uptake, structure and function of Hemoglobin Myoglobin. Hemogyanins and hemerythtin, model synthetic complexes iron, cobalt and copper. Electron Transfer in Biology- Structure and function of metalloproteins in electron transport processes, Cytochromes and ion-sulpher proteins, synthetic models. Nitrogenase- Biological nitrogen fixation, Mo-Nitrogenase spectroscopic and other evidences. Other hitrogenases and model systems:

UNIT-III BIO-ORGANIC CHEMISTRY

Introduction- Basic considerations, Proximity effects and molecular adaptation. Enzymes- Introduction and historical perspective, Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extractions and portrication, Fischer's lock and key and Keshland's induced Fit hypothesis, Concepts and identification of active site by the use of inhibitors, affinity labeling and enzyme medification by side-directed mutagenesis. Enzyme kinetics. Michaelis- Menten and Lineweaver- Burk plots. Reversible and irreversible inhibition.

UNIT-IV

Kinds of Reaction catalysed by Enzymes- Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer to sulphase, addition and elimination reactions, enolic intermediates in isomerisation reactions, Beta-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

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Co-Enzyme Chemistry- Cofactors as derived from vitamins, coenzymes, prosthetic groups, apo-enzymes structure and biological function coenzyme A thiamine pyrophosphate, pyridoxal phosphate, NAD+, NAD++, FMN, FAD, Lipoic acid. Vitamins B12 Mechanisms of reactions catalysed by above cofactors.

UNIT-V

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.

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

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Book Suggested-

- 1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg. University Science Book.
- 2. Bioinorganic Chemistry L. Bertoni, H.B. Gray, S.J. Lippard and J.S. Velentine, University Science books.
- 3. Inorganic Biochemistry Vol. Fand It Ed. GL Eichhron. Elsveier
- 4. Progress in Inorganic Chemistry Vol. 18 and 38 Ed. JJ Lippard Wiley.
- 5. Bioinorganic Chemistry: A Chemical approach to Enzyme action. Hormann Dugas and C Penny Springer Veralg.
- 6. Understanding Enzymes, Trayor Palmer Hall.
- 7. Enzyme Chemistry Impact and application Ed. Collin J Suckling. Chapmad and
- 8. Enzyme Mechanisms Ed M.I. Page and A Williams, Royal Society of Chemistry.
- 9. Fundamentals of Enzymology, N.C. Price and L. Sievens Oxford University Press.
- 10 Immobilised Enzyme- An introduction and application in Biotechnology Michael D TreVan John Wiley 11. Enzymetic Reaction Mechanisms: C Walah W.H. Freeman. 12. Enzyme structure and Mechanism — A Fersht, W.H. Freeman.

- 13. Blochemistry-The Chemical Reactions of living cells. DE Metzier. Academic press.
- 14. Principles of Biochemistry. A.L. Letinger, Worth Bublisher.

- 15. Biochemistry I. Stryer W.H. Freeman.
 16. Biochemistry J. Bavid Rawn, Neil Patterson.
 17. Biochemistry Voiet and Voiet, John Wiley.
 18. Outlines of Biochemistry, EE. Corn and PK Stumpt. John Wiley.
 19. Biochemistry, L. Stryer, W.H. Freeman.
 20. Biochemistry, J. David Rawn, Neil Patterson.

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- 21. Blochemistry- Voet & Voet John Wiley
- 22 Biochemistry- Jain & Jain, S. Chand
- 23. Bio-Inorganic Chemistry By Kalsi

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SEMESTER III GROUP- A INORGANIC CHEMISTRY PAPER- III ORGANOTRASITION METAL CHEMISTRY

UNIT-I

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

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UNIT- II

Compounds of transition Metal-Carbon multiple bonds. Alkylidenes, alkylidenes, low valent carbones and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

UNIT- III

Fransition Metal π – **Complexes**-Transition metal π -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features, import reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

UNIT-IV

Transition Metal Compounds with Bonds to Hydrogen-Transition metal compounds with bonds to hydrogen.

Fluxional Organometallic Compounds-

Fluxionality and dynamic equilibria in compounds such as ² olefin ² allyl and dienyl complexes.

UNIT- V

Homogeneous Catalysis-

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (excreaction) expalladation reactions, actions of C-H bond.

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M.Sc. CHEMISTRY

SEMESTER III GROUP- A INORGANIC CHEMISTRY PAPER- IV PHOTOINORGANIC CHEMISTRY

UNIT- I Basic of Photochemistry -

Absorption, excitation, photoshemical laws, quantum yield, electronically excited states-life times-measurements of the times, Flash photolysis, stopped flow techniques, Energy dissipation by radiative and non-radiative processes absorption spectra Franck-Cordon principle, photochemical states- primary and secondary processes.

UNIT- II Properties of Excited States-

Structure, dipole moment, acid-base strengths, reactivity, photochemical kinetics-calculation of rates of radiative processes, Bimolecular deactivation quenching,

UNIT- III 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- IV Ligand field Photochemistry-

Photo-substitution, photo-exidation and photo-reduction, lability and selectivity. Zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

Metal Complex Sensitizers-

Metal Complex sensitizer, electron relay, metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

UNIT- V Redox reactions by excited Metal Complexes

Energy transfer under conditions of weak interaction and strong interaction exciplex formation: Conditions of the excited states to be useful as redex reactants, excited electron transfer, metal complexes as attractive candidates (e. 2'-bipyridine and 1, 10-phenanthroline complexes), illustration of reducing and excited character of Rothenium^{2*} (bipyridal complex), comparison with fe (bipy)₃ role of spin-orbit coupling life time of these complexes. Application of redex processes of electronically excited states for catalytic purposes transformation of low energy reactants into high energy products, chemical energy into light.

Book Suggested-

- Principle and application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, 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 Age Internation.
- 5. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischaur, Willey.
- 6. Inorganic Photochemistry, J. Chem, Educ, Vol 60 No. 10, 1983.
- 7. Progress in inorganic Chemistry vol 30ed , S.J. Lippard, Wiley.
- 8. Coordination Chem Revs., 1981, Vol 39, 121, 131, 1975, 15, 321, 1990, 97, 313.
- Photochemistry of Coordination compounds, V. Balzan and V. Carassiti Academic Press.
- 10. Elements of Inorganic Photochemistry, G.J. Ferraudi Wiley.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER III GROUP-B ORGANIC CHÉMISTRY PAPER-III PHYSICAL ORGANIC CHÉMISTRY

UNIT - I

Concepts in Molecular orbital (MO) and Balance Bond (VB) Theory:

Introducation 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.

Quabtiative MO theory - Huckel molecular orbial (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 butadiene. methyl group.conjugation ethene. allyl. methane and configuration hyperconjugationaromaticity. valence bond (VB) diagrams.hyperconjugationaromaticity, valence bond (V8) 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.

UNIT - II

Solvation and Solvent Effects & Acids, Bases, Electrophiles, Nucleophiles, Catalysis: Qualitative understanding of solvent-solute effects on reactivity thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria, various emperical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Acid-base Dissociation, Electronic and structural Efects, acidity and basicity, acidity functions and their application, hard and soft acids and bases, nucleophilicity scales, nucleofugacity. The alpha-effect, Ambivalent nucleophiles. Acid-Bases catalysis-specific and General Catalysis. Bronsted catalysis, nucleophilic and electrophilic catalysis. Catalysis by non covalent binding-micellar catalysis.

UNIT - III

- (a) Principles of Reactivity: Mechanistic significance of entropy enthalpy and Gibb's free energy. Arrhenius equation transition state theory. Uses of activation parameters. Hammond's postulate Bell-Evans-Polanyi principle potential energy surface model. Marcus theory of electron transfer reactivity and selectivity principles.
- (b) Radical and Pericyclic Reactions: Radical stability, polar influences, solvent and steric effects a curve crossing approach to radical addition. Factor affecting barrier heights in additions regional reaction regional reaction. Reactivity specificity and periselectivity in perictions.

UNIT - IV

Nucleophillic and Electrophilic Reactivity:

Structural and electronic effects on S_N 1 and S_N 2 reactivity. Solvent effects.Kinetic isotope effects.Intramolecular assistance. Electron transfer nature of S_N 2 reactions. Nucleophilicity and S_N 2 reactivity based on curve-crossing model, relationship between polar and electron transfer reactions. S_{RN} 1 mechanism, electrophilic reactivity, general mechanism kinetic of S_E 2 Ar reaction, structural effects on rates and selectivity Curve-crossing approach to electrophilic reactivity.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

UNIT - V

Steric and Confornational Properties:

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

Book Suggested:

- 1. Molecular mechanics U Burkert and N.L. Allinger ACD Monograph 177, 1982.
- 2. Organic Chemists Book of Orbirals. L. Salem and W.L. Jorgensen, Academic Press.
- 3. Mechanism and Theory in Organic Chemistry, T.H.Lowry and K.C. Richardson, harper and Row.
- 4. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W.B. smith VCH. Weinheim.
- 5. Physical: Organic Chemistry, N.S. Isaacs. ELBS/ Longman.
- 6. Supramolecular Chemistry Concepts and Perspectives, J.M. lehn. VCH.
- 7. The physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-IV GROUP-B LABORATORY COURSE (SPECIAL) ORGANIC CHEMISTRY

200 marks

Note: Laboratory course with Group 'B' will be of 12 hrs duration spread over two days. The examinee will have to perform three experiments. These experiments will be of 40 marks each. 40 marks each will be allotted for viva-voce and Sessional work.

Qualitative Analysis

Separation, Purification and identification of the components of a mixture of binary organic compounds & mixture of three organic compounds.

Multi-step synthesis of Organic compounds (Three stage preparations. Preparation of pure crystalline product. By using any two following principals Conformation by melting point determination.)-

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

- 1. Photochemical reaction: Benzophenone- Benzopinacol- Benzoinacolone.
- 2. Beckmann rearrangement: Benzanilide from benzene, Benzene- benzophenone ,oxime-Benzanilide.
- 3. Benzilic acid rearrangement : Benzilic acid from benzoin, (Benzoin- Benzil- Benzilic acid)
- 4. Synthesis of heterocyclic compounds, Skraup synthesis: Preparation of quinoline from aniline, Skraup synthesis: Preparation of 2 phenyl-indole from phenyl hydrazine.
- 5. Sandmayer Reaction: Preparation of o chlorobenzoic acid from anthranilic acid.
- 6. Ultman reaction Preparation of N-Phenyl anthranilic acid from o-chlorobenzoic acid.
- 7. Preparation of Acridone from N-Phenyl anthranilic acid.
- 8. Prepration of pinitro aniline
- 9. Prepration of p bromo aniline
- 10. Prepration of methyl orange from aniline via sulphanilic acid.

Extraction of Organic compounds from Natural sources-

- 1. Isolation of caffeine from tea leaves
- 2. Isolation of casein from milk
- 3. Isolation of lactose from milk
- 4. Isolation of nicotine dipicrate from tobacco
- 5. Isolation of piperine from black pepper
- 6. Isolation of lycopene from tomatoes
- 7. Isolation of b-carotene from carrots.

Paper Chromatography

Separation and identification of the sugars, dyes and amino acids present in the given mixture of sugars, dyes and amino acids by paper chromatography and determination of RF values.

Spectroscopy:

Identification of organic compounds by the analysis of their spectral data (UV. IR. PMR, CMR & M) Spectrophotometric (UV/VIS) Estimations of

- 1. Amino acids
- 2. Proteins
- 3. Carbohydrates
- 4. Aspiri

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER-IV GROUP-B LABORATORY COURSE (SPECIAL) PHYSICIAL CHEMISTRY

- 1. Study of kinetics of exchange between ethyl lodide and the iodide ion.
- 2. Determination of the solubility product of lead iodide.
- 3. Determination of the dissociation constant of barium nitrate.
- Determination of relative strength of the acids by studying the hydrolysis of an ester.
- Study the hydrolysis of methyl acetate catalysed by HCI and equimolar ureal hydrochloride and hence the degree of hydrolysis of the salt.
- 6. Investigate the inversion of can-sugar in presence of an acid. Determine also the energy of activation of the reaction.
- Study in inversion of can-sugar in presence of HCL and H₂SO₄ and hence determine the relative strength of the acids.
- 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.
- Study the kinetics of hydrolysis of tertiary amyliodide, and determine the order and energy of activation of the reaction.
- 10. Investigate the reaction between H₂O₂ and HI.
- 11. Study the kinetics of decomposition of benzene diazonium chloride at different temperatures.
- 12. Study the kinetics of reaction between K2S2Oa and KI.
 - (a) Determine and rat constant and order of reaction.
 - (b) Study of influence of ionic strength on the rate constant.
- 13. Investigate the kinetics of autocatalytic reaction between KMno4 and Oxalic acid.
- 14. Determination of order of reaction between bromic acid and hydrobromic acids.
- Determination of concentration finding in a given sample (KI) by isotope dilution technique.
- 16. Determination of effect of-
 - (a) Change of temperature.
 - (b) Change of concentration.
 - (c) lonic strength of the media on the velocity constant of hydrolysis of an ester.
- 17. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (lodide ion is exidised by persulphate ion.)
- 18. Investigate the adsorption of oxalic acid from aqueous solution by activated charcoal and verify Frenndlish and Langmuir's adospriton isotherms.
- 19. Determine adsoption isotherms of acetic acid from aqueous solution by charcoal.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER IV
GROUP C
PHYSICAL CHEMISTRY
PAPER III
LIQUID STATES

تعاور العارب فالعول بكالتنابية المحموصة

UNIT-I

General properties of Liquids

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

b) A classical partition function for liquids, correspondence principle, configuration,

integral, configuration properties.

II-TIMU

Theory of liquids

Theory of liquids, partition function, method or model approach; single cell models, communal energy and entropy, LTD Model, significant structure model.

UNIT-III

Distribution function and Related Equations

Radial distribution method, equation of state in terms of RDF. Molecular distribution functions, pair function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, clusters expansion.

UNIT-IV

Methods for Structure Determination and Computational Techniques

Spectroscopic techniques for liquid dynamic structure studies. Neutron and X-ray scattering spectroscopy. Computation Techniques-Monte Carlo and molecular dynamics methods.

UNIT- V

Super cooled and lonic Liquids

Super cooled and tonic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in super cooled liquids.

Books Suggested

- 1. An Introduction to Liquid State, P.A. Egelstaff, Academic Press.
- 2. The Dynamic Liquid State A.F.M. Barton, Longman.
- 3. Introduction to Statistical Thermodynamics, T.L. Hill, Addison Wiley.
- 4. The Liquid State J.A. Pryde.
- 5. Significant Liquid Structures, H. Eyring and M.S. John.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER IV GROUP C PHYSICAL CHEMISTRY PARER IV COMPUTATION CHEMISTRY

UNIT - I

Fortran/c 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 subtopic considering the background of students, available time etc.

Solution of Equations-Bisection, regular falsi, Newton -Raphosn and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.

Linear Simultaneous Equations-Gassian elimination, Gauss -Seidel method, Gauss-Jordan method, Pivoting strategy. Errors and ill conditioning.

UNIT - II

Eigen values and Matrix Diagonalization-Jacobi and Householder methods, analysis or errors.

Interpolation-Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation, Polynomial wiggle problem.

UNITABILITY

Numerical Differentiation-Solution of simple differential equations by taylor series and Runge-Kutta methods:

Numerical Integration-Newton-Cotes formulae, romberg intergration, errors in integration formulae.

The Students should develop computer programs for some of the above numerical methods.

UNIT - IV

Running of Advanced Scientific Packages-The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology, ab initio quantum chemical packages such as GAUSSIAN/GAMES. With carefully designed exercises for illustrating various features of the packages. Semi-empirical/Dynamics/simulation packages such as MOPAC, CHARM, AMBER; QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design, etc.

UNIT-V

Introduction to Networking and using Internet -Project- The students will develop utilities such as analysis of spectre, simulation programmes which will supplement laboratory or theory exercises in physical organic inorganic chemistry or biochemistry. This list in only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out.

Book Suggested

- 1. Computational Chemistry, A.C. Norris, John Wiley.
- 2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall,
- 3. Numerical Analysis, C.E. Frogberg, Macmillan.
- 4. Numerical Analysis A Practical Approach, M.J. Maron John Wiley.
- 5. Numerical Methods for Scientists and Engineers, H.M. Antia, Tata McGraw, Hill.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

SEMESTER IV GROUP C PHYSICAL CHEMISTRY LABORATORY COURSE (SPECIAL)

200 marks

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.

Thermodynamics

- (i) Determination of partial molar volume of solute (e.g., KCI) and solvent in a binary Mixture.
- (ii) 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.

Spectroscopy

- (i) Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b0 micellar media.
- (ii) Determination of stoichiometry and stability constant of inorganic (e.g. ferric salicylic acid) and organic (e.g. amine-iodine) complexes.
- (iii) Characterization of the complexes by electronic and IR spectral data.

Polarography

- (i) Estimation of Pb2+ and Cd2+ /Zn and Ni2+ icon in a mixture of Pb2+/Zn+ and Ni2+ by Polarography.
- (ii) Determination of dissolved oxygen in aqueous solution of organic solvents.

Electronic

This lab course will have theory as well as practical and the lectures shall be delivered during lab hours.

Basic Electronics

Notations used in an electric circuit, study of electronic components and colour codes, conversion of chemical quantities into electrical quantities. Transducer, illustration with electrodes, thermocouples and thermostats. Passive components: Resistors, capacitors and inductors with some emphasis on solid state properties of materials. Net works of resistors. The venin's theorem, superposition theorem, loop analysis R C circuits, L R circuits Illustration of the use of the circuits in NQR spectroscopy, Mossbauer spectroscopy, cyclic voltametry and in power supplies as filter 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. Transistors: An extension of p-n junction to p-n-p and n-p-n transistors. Characteristics of circuits. Dereliction pairs, differential amplifiers.

Operational Amplifiers

Ideal characteristics; inverter, summer, integrator, differentiator, voltage follower, illustrative use of operational amplifiers. Introduction to Fourier transform in instrumentation.

SEMESTER SYLLABUS M.Sc. CHEMISTRY

List of Experiments in Electronics

- 1. Measurements of resistance with multimeter
- 2. To measure the resistance of the given ammeter
- 3. Voltage measurement with CRO
- 4. Familiarising with CRO
- 5. Use of a Wheatstone Bridge for accurate measurement of resistance
- 6. Capacitor as a charge storage device
- To study the behaviour of parallel charged capacitors in series charged capacitors
 placed in parallel
- 8. The use of LCR-Bridge
- 9. Response characteristics of RC network
- 10. Response characteristics of LR network
- 11. Response characteristics of LCR network
- 12. Verification of Kirchoff's law
- 13. To study the Lissaiou's figures
- 14. Measurement of e.m.f. with thermocouple
- 15. To plot the characteristic curve of a diode
- 16. Half-wave and full-wave rectifier
- 17. Clipping and clamping circuits.
- 18. Capacitor filter for full-wave rectifier
- 19. Voltage doubles. Zeher stabilized bipolar power supply
- 20. Transistor characteristics
- 21. Differential amplifier
- 22. Transistor amplifier
- 23. Transistor amplifier
- 24. Introduction of an operational amplifier as a voltage follower
- 25. Op-Amp as non-inverting and inverting amplifier
- 26. Simple integration differentiation with Op-Amp 741
- 27. Op-Amp as comparator
- 28. Designing and fabrication of a printer circuit board
- 29. Setting up of a thermostat Constant temperature bath
- 30. Four-probe method for resistivity measurement

Books Suggested

- Inorganic Experiments, J. Derek Wootlins VCH.
- 2. Micro scale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.
- 3. Practical Inorganic Chemistry, G. Marr and B.W. Rockett, Van Nostrand
- 4. The Systematic Identification of Organic Compounds, R L. Shriner and D. Y. Curtin.
- 5. Semi micro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett
- 6. Experimental Organic Chemistry M. P. Doyle and W.S. Mungail
- 7. Small Scale Organic Preparations, P.J. Hill.
- 8. Organ metallic Synthesis, J.J. Fisch and R.B. King, Academic.
- Experimental Physical Chemistry, D.P. Shoemaker C.W. Garland and J.W. Niber, McGraw Hill Inter science.
- 10. Findlay's Practical Physical Chemistry revised B.P. Levitt, Longman.
- 11. Experiments in Physical Chemistry, J.C. Ghosh Brarati Bhavan.