M. Sc. Syllabus of Subject Chemistry

M. Sc. Chemistry

(Four-semester course)

Semester	Paper	Course No.	Course	Periods/ Week	Total periods	Marks
1st	I	CH-411	Inorganic Chemistry-I	4	45	50
	II	CH-412	Organic Chemistry-I	4	45	50
	III	CH-413	Physical Chemistry-I	4	45	50
	IV	CH-414	Physical methods in Chemistry-I	4	45	50
2nd	IX	CH-421	Inorganic Chemistry-II	4	45	50
	X	CH-422	Organic Chemistry-II	4	45	50
	XI	CH-423	Physical Chemistry-II	4	45	50
	XII	CH-424	Principles of Spectroscopy-II	4	45	50
	V	CH-401	Laboratory Course-I	6	132	50
	VI	CH-402	Laboratory Course- II	6	132	50
	V11	CH-403	Laboratory Course- III	6	132	50
	V111	CH-404	Laboratory Course- IV	6	132	50

Instructions

1. M.Sc. I semester 4 Theory papers of 200 marks.

2. M.Sc. II semester 4 Theory papers of 200 marks and 4 Laboratory Course of 200 marks.

Note:

I] Each Laboratory Course of 6 Hrs duration should be completed in 6 Hrs per day.

II] Each student have to give one Seminar in each semester [5 marks]. The marks to be given in fourth semester[internal marks 20].

M. Sc. First Year, Semester-I
Inorganic Chemistry - I
Paper: I, (CH-411)

Marks: 50 **45P**

1. **Reactions of metal complexes** 15 periods
(Part I)

1.1 a. Introduction
b. Lible and Inert complexes
c. VBT explanation of libility and inertness.
d. Taube's explanation of libility and inertness.

1. 2 a. Ligand substitution reactions.
b. SN^1: substitution, nucleophilic, unimolecular mechanism (Dissocitive mechanism) : Introduction, Characteristics, Example.

c. SN^2: substitution, Nulcleophilic, Bimolecular Mechanism (Associative mechanism): Introduction, Characteristics, Example.
d. SN^1CB : Substitution Nucleophilic Unimolecular Conjugate Base Mechanism : Characteristics, Example.
e. Anation Reaction.

1.3 Electron-transfer reactions.
(Redox reaction)

a. Introduction with example.

b. Outer sphere mechanism, tunneling mechanism, essential requisite for electron transfer, factors which favour outer sphere electron transfer reactions.

c. Inner-sphere mechanism, characteristics, example, proof for inner-sphere mechanism, inner sphere mechanism and bridging ligand, inner sphere mechanism and electronic configuration.
(For this chapter use **concise coordination chemistry by R. Gopal, V. Ramlingam, Vikas Publishing House Pvt. Ltd**.).

2. **d-Metal organometallic Chemistry** 15 P

2.1 a. Introduction

b. Bonding - Stable electronic configuration, 18 electron compound, 16 electron square planar compounds, electron count preference, electron counting and oxidation states, neutral ligand method donor pair method and nomenclature.

2.2 Ligands

Carbon monoxide, phosphines, dinitrogen and nitrogen monoxide, cyclopentadiene, cyclopentatriene and carbene.

2.3 Compounds

a. d block carbonyl

b. Homoleptic carbonyl.
Definition, Synthesis, properties, oxidation & reduction of carbonyl, metal carbonyl basicity and spectroscopic properties of carbonyl compounds.

c. Metallocenes.

Introduction, structure of metallocene, properties of metallocene, preparation method of metallocene. Ferrocene :- Preparation, structure, Aromatic character.

d. Metal-metal bonding and cluster : Introduction, structure of cluster, electron counting in cluster, synthesis of cluster.

e. Reactions of Organometallic Compounds:
Ligand substitution, oxidative addition and reductive elimination.

(For this chapter use **5th edition of Shriver Atkins - Inorganic Chemistry, Oxford University Press).**

3. **Spectral and Magnetic Characteristics of Metal Complexes**. 15 P

a. Introduction
b. Term Symbol, Rules for determining the ground state term symbol for d^n configuration according to L-S. Coupling.
c. Microstates. Calculation of number of microstates.
d. Correlation diagram of d^1 & d^9, d^2 & d^8 in octahedral & tetrahedral field.
e. Tanabe-Sugano diagram of d^2 & d^3 configuration of an octahedral environments.
f. Calculation of Reacah parameter such as Dq, B, and β.
g. Charge transfer spectra : Types of transition, MOT for tetrahedral complex (ML_4) showing possible ligand-metal charge transfer transition. ML_6 octahedral complex showing metal to ligand charge transfer transitions.
h. Magnetic moment of transition metal ions having d^1 to d^9 configuration.
i. Spin cross over.

Reference Books :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
4. Magneto chemistry, R.L. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
6. Advanced Inorganic Chemistry : Satyaprakash, J.D. Tuli, Version I S.K. Basu and R.D. Madan.
7. Advanced Inorganic Chemistry : Vol. I and II Gurudeep Raj.

8. Concise Inorganic Chemistry : J.D. Lee.
9. Principles of Inorganic Chemistry : Puri, Sharma and Kalia.
10. Inorganic Chemistry (Principles, structures and reactivity) (4th Edition): J.E. Huheey, E.A. Keitler and R.L. Keitler.
11. Inorganic Chemistry 3rd Edition : G.Y. Miessler and D.A. Tarr.
12. Selected topics in Inorganic Chemistry : W.U. Malik, J.D. Tuli and R.D. Madan.
13. Chemistry of the elements : N.N. Greenwood and A. Earnshaw.
14. Symmetry and Spectroscopy of molecules : K. Veera Reddy.
15. Inorganic Chemistry : Attkin and Shriver.
16. Some Aspects of Crystal Filed Thoery : T.M. Dunn, D.S. Mcclure and R.G. Person.
17. Introduction to Ligand Files : B.N. Figis

M. Sc. I Semester
Organic Chemistry I
Paper: II (CH - 412)

Marks: 50 **45P**

1. Reaction Mechanisms: Structure and Reactivity. **10P**

a) Types of mechanism, types of reaction, Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's postulate. Potential energy diagrams, Transition state and intermediates.

b) Determining mechanism of a reaction: Product analysis, kinetic studies, stereo-chemical outcome, detection and trapping of intermediates, cross over experiments, kinetic isotope effect- primary kinetic and secondary kinetic isotope effect.

c) Effect of structure on reactivity–The Hammett equation and linear free energy relationship, Substituents and reaction constants. Taft equation.

d) Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, Energy level of π-molecular orbitals, Annulenes, Antiaromaticity, Homoaromaticity.

e) Reactive intermediates: Generation, Structure and stability of carbocations, Carbanions, Free radicals, Carbenes and nitrenes. Types of reagents.

2. Nucleophilic Substitution: **12P**

a) Aliphatic Nucleophilic Substitution:

1. The SN^2, SN^1, mixed SN^1 and SN^2 and SET mechanism. The neighbouring group mechanism, Neighbouring group participation by π and σ-bonds, Anchimeric assistance. The SN_i mechanism.
2. Nucleophilic substitutions at an allylic, Aliphatic and a vinylic carbon.
3. Reactivity effects of substrate structure, Attacking nucleophile, Leaving group and reaction medium.

b) Aromatic nucleophilic Substitution:

SN^{Ar}, SN^1, Benzyne and SNR^1 mechanism. Reactivity: Effect of substrate, Leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser and Smiles rearrangements.

3. Electrophilic Substitution: **11P**

a) Aliphatic Electrophilic Substitution :Bimolecular mechanism–SE^2 and SE_i. The SE^1 mechanism, Electrophilic substitution accompanied by double bond shift. 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.Quantitative treatment of reactivity in substrates and electrophiles.Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

4. Photochemistry: **12P**

Principles–photochemical theory, electronic excitation, singlet and triplet states, Jablonski diagram. Energy transfer, quantum efficiency.

a) Photochemistry of carbonyl compound: 1) Photoreduction, 2) Norrish type–I & II, 3) Paterno-Buchi reaction.
b) Photochemistry of α, β-unsaturated ketones.
c) Photochemistry of olefins: cis-trans isomerism.
d) Miscellaneous photochemical reaction: Photo-fries reaction of anilides, Photo-rearrangements, Barton reaction singlet molecular oxygen reaction photochemical formulation of smog photo-degradation of polymers, photochemistry of vision, nπ - pπ rearrangement.

Reference Books:

1. Advanced Organic Chemistry-Reaction Mechanism and structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S.P. Singh, Macmillan.
9. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.
10. Advanced Organic Chemistry – Jagdamba Singh and L.D.S. Yadav.
11. Advanced Organic Chemistry Reaction and Mechanism– Maya Shanker Singh

M. Sc. First Year, Semester-I
Physical Chemistry
Paper: III (CH – 413)

Marks: 50 **45P**

1. Quantum Chemistry: **15P**

A. Introduction to Exact Quantum Mechanical Results:

a)The postulates of quantum mechanics.

b) Schrödinger equation in Laplacian and Hamiltonian form. Significance of Eigen – values and Eigen functions. Significance of Ψ and $\Psi^{2.}$

c) Discussion of solutions of the Schrödinger equation to

i. Particle in one dimensional box,
ii. Particle in three dimensional box,
iii. Harmonic oscillator,
iv.The rigid rotator and
v. Hydrogen and Hydrogen like systems.

d) Orthogonality and normalisation of wave functions.

e) Numericals on (c) and (d).

B. Approximate Methods:

a) The variation theorem, linear variation principle.

b) Perturbation theory (first order and non degenerate).

C. Angular Momentum:

a) Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum.

b) Spin, anti-symmetry and Pauli's exclusion principle, commutation relation, zeeman splitting, Spin orbital coupling and R-S couplings.

c) Operator using ladder operators, addition of angular momentum.

Home assignment for students:

Applications of variation method and perturbation theory to the Helium atom.

2. Phase Rule: **04P**

a) Recapitulation of phase rule and terms involved in it.

b) Three component system: representation of ternary systems.

c) Partially miscible three liquid systems:-1) system composed of three liquid components, one partially miscible pairs, two partially miscible , three partially miscible pairs. 2) System composed of two solid and a liquid components:- formation of eutectic systems, crystallisation of pure components only, formation of binary compounds, one double salt formation .

Home assignment for students: formation of binary compounds hydrate formation, formation of ternary compounds, formation of solid solutions, partially miscibility of phases.

3. Thermodynamics: **15P**

A. Classical Thermodynamics:

a) Brief resume of concepts of laws of thermodynamics. Free energy and entropies.

b) Partial molar, partial molar free energy chemical potential, partial molar volume and partial molar heat content and their significances. Determinations of these quantities.

c) Concept of fugacity and determination of fugacity by graphical method and from equation of state.

d) Non-ideal systems : Excess functions for non-ideal solutions.

e) Activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients by 1) solubility 2) E.M.F. method.3) vapour pressure method, Ionic strength.

B. Statistical Thermodynamics:

a) Concept of distribution, thermodynamics probability, ensemble averaging, postulates of ensemble avaranging. Canonical, grand canonical and micro-canonical ensembles.

b) Partition functions: Translational, rotational, vibrational and electronic partition functions. calculation of thermodynamic properties in terms of partition functions.

c) Applications of partition functions.

Home assignment for students: a) Corresponding distribution laws (Max well-Boltzaman distribution law b) Heat capacity behaviour of solids –chemical equilibria constant in terms of partition functions.

C. Crystallography 03 Hrs

a) semiconductors, N and P type, effect of temperature on N and P type semiconduction.

b)Packing of uniform spears, octahedral and tetrahedral voids(holes), close packing of spear.

c) Isomorphism, lattice energy and born haber cycle.

4. Electrochemistry I 08 Hrs.

a) Anomaly of strong electrolytes, Deby-Huckel theory, Onsager equation, & its verification wine effect, Deby falkenhagen effect, ion solvent, intractions.

b) Thermodynamics of electrified interface equation, Derivation of electro capillary ,Lippmann equation (surface excess)

c) Structure of electrified interfaces equation, Electrical double layer, Theories of structure of Electrical double layer. Helmoholtz-perrin. Gouy-Chapman theory, Stern's theory.

Books Suggested

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

M. Sc. I Semester
Physical Method in Chemistry
Paper: IV (CH - 414)

Marks: 50 **45P**

1. Symmetry and Group Theory in Chemistry **12P**

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonfiles symbols, representations of groups by matrices (representation of the C_n, C_{nv}, C_{nh}, D_{nh} etc . groups to be worked out clearly.) Character of a representation . The great orthogonality theorem (without proof) and its importance. Character tables C_1h, C_2v, C_3v and their use.

2. Computer for Chemist **20P**

A. Introduction to computers and computing:

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

B. Programming in Chemistry:

Development of small computer codes involving simple formulae in chemistry, such as Vander Waal's equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy from experimental data. Linear simultaneous equation to solve secular equation within the Hückle theory. Elementary structural features such as bond lengths, bond angles of molecules extracted from data base such as Cambridge data base.

3. X-ray Diffraction **9P**

Bragg condition. Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramachandran diagram. Numerical on Braggs equation. $n\lambda=2d\text{Sin}\theta$

4. Electron Diffraction: **2P**

Scattering intensity vs. Scattering angle,Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules with suitable examples.

Home assignment for students: Low energy electron diffraction and structure of surfaces.

5. Neutron Diffraction **2P**

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. **Home assignment for students:** Elucidation of structure of magnetically ordered unit cell, applications.

Books Suggested

1. Physical Methods in Chemistry - R.S. Drago, Saunders College.
2. Chemical Applications of Group Theory - F.A. Cotton.
3. Basic Principles of Spectroscopy - R.Chang, McGraw Hill.
4. Computers and common Sense, R. Hunt and J. Shelly, Prentice Hall.
5. Computational Chemistry, A. C. Norris.
6. An introduction to digital computer design, V.Rajaram and T. Radhakrishnan, Prentice Hall.
7. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.

M. Sc. II Semester

Inorganic Chemistry-II
Paper: IX (CH - 421)

Marks: 50 **45P**

1. **Reaction of Metal Complexes** 08 Period
(Part II)

   a. Substitution reactions of sqare-planar complexes.
   b. Evidence for associative type SN^2 mechanism.
   c. Trans effect, applications of trans effect.
   d. Theories of trans effect, the polarization theory, evidences in favour of the polarization theory, defect of this theory, the Pi-bonding theory.
   e. Cis effect.

   (For this chapter use **concise coordination chemistry by R. Gopal, V. Ramlingam, Vikas Publishing House Pvt. Ltd**.).

2. **Catalyst.** 15 P.

   a. Introduction, General principle and mechanism of catalytic rea^n. Types of catalysts.
   b. Homogeneous Catalysis : Hydrogenation of alkenes, Hydroformulation, Methanol Carbonylation, Wacker oxidation of alkenes, Palladium-catalysed C-C bond forming reaction, Heterogeneous catalysis : The nature of Heterogeneous catalysts, amonia synthesis, Sulfur dioxide oxidation, Fischer-Tropsch Synthesis, Alkene Polymerization, New directions in heterogeneous catalysis such as Tethered catalysts.

   (For this chapter use **5th edition of Shriver Atkins - Inorganic Chemistry, Oxford University Press)**

3. **Bioinorganic Chemistry:** 12 P
   a. Biological importance of essential and non essential elements.
   b. Na/K Pump.
   c. Metalloporphyrins : Structure of porphyrin molecule. **Hameoglobin :** Structure, function of haemoglobin. **Myoglobin :** Structure & function. Difference between haemoglobin & Myoglobin. **Chlorophyll** : Structure & function, Photosynethesis PS-I & PS-II.
   d. Electron carrier proteins in biological system :
      i. Iron sulfur proteins - Rubredoxin, ferrodoxin.
      ii. Cytochrome : Structure & function.
      iii. Iron storage protein : Ferritin.
      iv. Iron transporting biomolecule : Transferrin.
   e. Biological enzymes : Nitrogenase and Superoxide dismuthases.
   f. Vitamin B_{12} (Cynocobalanine), structure and function.

   (Inorganic Chemistry (Principles, structures and reactivity) (4th Edition): J.E.Huheey, E.A. Keitler and R.L. Keitler.)

4. **The Chemistry of elements in Medicine**. 04 P.
   a. Introduction
   b. Chelation therapy.
   c. Cancer treatment.
   d. Anti-arthritis drugs.
   e. Imaging agents.
   (For this chapter use **5th edition of Shriver Atkins - Inorganic Chemistry, Oxford University Press**).

5. **Structure of Ionic Solids** : 06 P
   a. Introduction, relation between limiting radius ratio, coordination numbers and shape.
   b. Ionic structure of Nacl, rutile structure of Tio2, β-crstobalite strucutre of SiO2, and layer structure of CdI.
   c. Stoichiometric defects : Introduction, schottky defect, Frenkel defects.
   d. Non stoichiometric defects : Metal excess defect - F-Centres, Intertitial ions and electrons. Metal deficiency defect - Positive ion absent, extra interstitial negative ions.
   e. Semiconductors : Introduction, N & P types of semiconduction.
   (Concise Inorganic Chemisstry 5th edition, J.D. Lee).

Reference Books :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
4. Magneto chemistry, R.L. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
6. Advanced Inorganic Chemistry : Satyaprakash, J.D. Tuli, Version I S.K. Basu and R.D. Madan.
7. Advanced Inorganic Chemistry : Vol. I and II Gurudeep Raj.
8. Concise Inorganic Chemistry : J.D. Lee.
9. Principles of Inorganic Chemistry : Puri, Sharma and Kalia.
10. Inorganic Chemistry (Principles, structures and reactivity) (4th Edition): J.E. Huheey, E.A. Keitler and R.L. Keitler.
11. Inorganic Chemistry 3rd Edition : G.Y. Miessler and D.A. Tarr.
12. Selected topics in Inorganic Chemistry : W.U. Malik, J.D. Tuli and R.D. Madan.
13. Chemistry of the elements : N.N. Greenwood and A. Earnshaw.
14. Symmetry and Spectroscopy of molecules : K. Veera Reddy.
15. Physical Chemistry through Problems : Dogra and Dogra.
16. Inorganic Chemisstr : Attkin and Shriver.
17. Elements of Magnetochemistry : A. Samal and R.L. Datta.
18. Some Aspects of Crystal Filed Thoery : T.M. Dunn, D.S. Mcclure and R.G. Person.
19. Introduction to Magnetochemistry : Alan Earnshaw.
20. Introduction to Ligand Files : B.N. Figgis.

M. Sc. II Semester
Organic Chemistry II
Paper: X (CH - 422)

Marks: 50 **45P**

1. Addition Reactions: **12P**

A] Addition to Carbon – Carbon Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regioselectivity and chemoselectivity, orientation and reactivity. Stereochemistry addition reaction- X_2 and HX in (E)-but-2-ene, (Z)--but-2-ene, fumaric acid, and cyclopentene. Addition to cyclopropane ring.Hydroboration, Michael reaction.Sharpless asymmetric Epoxidation.

B] Addition to Carbon – Hetero Multiple Bonds:

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, Organo-zinc and organo-lithium reagents to carbonyl and unsaturated carbonyl compounds.

Mechanism of Wittig reaction, Mannich, Benzoin, and Stobbe reaction.

2. Elimination Reaction: **4P**

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 group and the medium. Mechanism and orientation in pyrolytic elimination.

3. Pericyclic Reactions: **15P**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-haxatriene 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 cheleotropic reactions.

Sigmatropic rearrangements: Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3 and 5,5-Sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements.

4. Stereochemistry: **14P**

a) Stereo chemical principles: Enantiometric relationships, Distereomeric relationships, R and S, E and Z nomenclature, Dynamic stereochemistry, Prochiral relationships.Homotopic,enantiotopic, distereotopic groups and faces. Stereo-specific and stereo-selctive reactions.

b) Introduction of optical activity in absence of chiral carbon (Biphenyls, Spiranes, Allenes).

c) Conformational Analysis: Open chain compounds containing two chiral centers, Mono and dimethyl cyclohexane, cyclohexane-1,4-diol.Inter conversion of different projections (sawhorse-newman-fischer projections) Conformation of alpha and beta glucopyranose.

Reference Books:

1. Advanced Organic Chemistry-Reaction Mechanism and structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S.P. Singh, Macmillan.
9. Advanced Organic Chemistry – Jagdamba Singh and L.D.S. Yadav.
10. Advanced Organic Chemistry Reaction and Mechanism– Maya Shanker Singh.
11. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
12. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.

M. Sc. II Semester
Physical Chemistry II
Paper: X1 (CH - 423)

Marks: 50 **45P**

1. Surface Chemistry: 18P

A. Adsorption: a) Surface tension, capillary action, pressure difference across curved surface (Laplace equation).

b) Gibbs adsorption isotherm.

c) BET equation and estimation of surface area.

d) Surface films on liquids (Electro-kinetic phenomenon) and catalytic activity at surfaces.

Home assignment for students: Kelvin equation for vapour pressure of droplets.

B. Micelles: a) Surface active agents, classification of surface active agents.

b) Micellisation, hydrophobic interaction, critical miceller concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellisation - phase separation and mass action models.

Home assignment for students: solubilisation, micro emulsion reverse micelles.

C. Macromolecules: a) Polymers - definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers.

b) kinetics of polymerization, mechanism of polymerization.

c) Difference between polymers and macromolecules.

d) Molecular mass, number and mass average molecular mass, molecular mass determinations by i) osmometry, ii) viscometry, iii) diffusion and iv) light scattering methods.

Home assignment for students: Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

2. Electrochemistry-II: 9P

a) Over potential, types of over potentials.

b) Exchange current density, Derivation of Butler-Volmer equation, Tafel plot.

c)Semi conductor interface. Theory of double layer at Semi conductor , electrolyte solution interface , effect of light at semiconductor, Solution interface.

d)Polarography, Theory, instrumentation, working and applications of the technique.

e) Introduction to corrosion, homogenous theory, forms of corrosion, Corrosion monitoring and prevention methods

Home assignment for students:

a) Quantum aspect of charge transfer at electrodes –solution interfaces,quantisation of charge transfer, tonnelling

b) Electro catalysis influence of various parameters. Hydrogen electrodes,

c) Biochemistry, Threshold membrane phenomenon,Nernst-Plank equation.

3. Chemical Dynamics: 18P

a) Methods of determining rate laws – i) Differential method and ii) Fractional change method.

b) Theories of reaction rates – i) collision theory of reaction rates, steric factor, ii) Transition state theory, thermodynamic formulation of TST.

c) Ionic reactions, kinetic salt effects.

d)Dynamic chain (Kinetics of the reactions, thermal/photochemical) – i) pyrolysis of acetaldehyde , ii) decomposition of ethane, iii) hydrogen-chlorine reaction, iv) hydrogen-bromine reaction.

e) Oscillatory reactions (Belousov-Zhabotinsky reaction).

f) Enzyme catalysis, kinetics of enzyme reactions, Michalis - Menten equation.

g) General features of fast reactions, study of fast reaction by flow method. Flash photolysis and the nuclear magnetic resonance method.

h) Dynamics of unimolecular reactions - i) Lindemann hypothesis ii) Hinshelwood theory iii) K-R-R treatment and iv) slater's theory .

i) Numricals on (a) and (b).

Home assignment for students: a) Steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. b) Dynamics and molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution.

c) Dynamics of unimolecular reactions (Rice-Ramsperger-Kassel - Marcus [RRKM] theory of unimolecular reactions.)

Books Suggested

1 Physical Chemistry -P.W. Atkins, ELBS.
2 Introduction to Quantum Chemistry -A.K.Chandra,Tata McGraw Hill.
3 Quantum Chemistry - Ira N.Levine, Prentice Hall.
4 Coulson's Valence -R. McWeeny ELBS.
5 Chemical Kinetics -K.J.Laidler, McGraw Hill.
6 Kinetics and Mechanism of Chemical Transformations -J.Rajaraman and J.Kuriacose, Macmillan.
7 Micelles, Theoretical and Applied Aspects - V.Moroi, Plenum
8 Modern Electrochemistry Vol.I & II, J.O.M. Bockris & A.K.N. Reddy, Plenum
9 Introduction to Polymer Science - V.R.Gowarikar, N,V.Vishwanathan & J.Sridhar, Wiley Eastern.
10 Advanced physical chemistry – J.N. Gurtu & A. Gurtu, A Pragati Edition,

M. Sc. II Semester
Principles of Spectroscopy
Paper: X11 (CH - 424)

Marks: 50 **45P**

1. Unifying Principles: 7P

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.

Home assignment for students: Born-Oppenheimer approximation rotational, vibrational and electronic energy levels.

2. Mircowave Spectroscopy: 2P

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

Home assignment for students: Applications of Mircowave Spectroscopy.

3. Vibrational Spectroscopy: 10P

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

B. Raman Spectroscopy: Classical and quantum theories of Raman Effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman Spectroscopy.

Home assignment for students: Coherent anti Stokes Raman Spectroscopy (CARS.)

4. Electronic Spectroscopy 10P

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

B. Molecular Spectroscopy: Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radioactive and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

C. Photoelectron Spectroscopy: Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.

Home assignment for students: Auger electron spectroscopy -basic idea.

5. Magnetic Resonance Spectroscopy: 16P

A. Nuclear Magnetic Resonance Spectroscopy:

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements. Factors influencing chemical shift. Deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A_2B_2 etc.) spin decoupling; basic ideas about instrument. NMR studies of

nuclei other than proton - ^{13}C and ^{19}F. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Home assignment for students: . NMR studies of nuclei other than proton - ^{31}P

B. Electron Spin Resonanace Spectroscopy:

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

C. Nuclear Quadrupole Resonance Spectroscopy:

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant splitting. Applictions.

Books Suggested

1. Modern Spectroscopy - J.M. Hollas, John Wiley
2. Applied Electron Spectroscopy for Chemical Analysis Ed.H.Windawi & F.L.Wo.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. Introduction to molecular Spectroscopy - G.M.Barrow, McGraw Hill.
6. Basic Principles of Spectroscopy - R.Chang, McGraw Hill.
7. Theory and Applications of UV Spectroscopy - H.H.Jaffe & M.Orchin,IBH-Oxford.
8. Introduction to Phoroelectron Spectroscopy - P.K.Ghosh, John Wiley.
9. Introduction to Magentic Resonance - A.Carrington & A.D.Maclachalan, Harper & Row.

M. Sc. I Semester
Laboratory Course I
Paper: V (CH - 415) (Inorganic Chemistry)

Marks: 50 **132P**

1. Record and viva voce 05 Mark

2. Detection of three acidic and three basic radicals from a given salt mixture. Report the spot test of radicals.
(At least five mixtures) 15Mark

3. Preparation of metal complexes and characterized by spectral analysis.

   a. Mercury tetra thiocyanato Cobalt(II)
   b. Ammonium tetrathiocyanatodiammine Chromate(II) (Reineck's salt)
   c. Potassium trioxalato ferrate(III)
   d. Cis -potassium dioxalato diaquo chromate(III)
   e. Bis(dimetyl glyoxime) Nickel (0) Complex
   f. Hexammine Nickel(II) Chloride
   g. Tris(Acetyl acetanato) Magnease(III)
   h. Prussian blue complex.
   i. Bis (Acetylacetone) oxovanadium(IV) Complex.

   15Mark

4. Separation and estimation of one of the metal ion volumetrically.

   a. Fe^{+3} and Zn^{+2}

   b. Ni^{+2} and Cu^{+2}

   c. Cu^{+2} and Ba^{+2}

   d. Ni^{+2} and Zn^{+2}

   e. Cu^{+2} and Fe^{+2}

   f. Ba^{+2} and Mg^{+2}

   15Mark

M. Sc. I Semester
Laboratory Course II
Paper V1: (CH - 416) (Organic Chemistry)

Marks: 50 **132P**

1. Techniques:

a) Simple distillation.
b) Steam distillation.
c) Thin layer chromatography.
d) Column chromatography.

2. Qualitative analysis:

a) Separation, Purification, sample submission and identification of compounds of binary mixture (one solid and one liquid) by chemical method (Any six).
b) Separation, Purification, sample submission and identification of compounds of binary mixture (solids) physical method (Any three).

3. Preparations (Double stage), (Any Four):

a) Phthallic anhydride-phthalimide-Anthranilic acid.
b) Acetophenone-oxime-Acetanilide.
c) Phthallic anhydride-o-benzoyl benzoic acid-Anthraquinone.
d) Chlorobenzene-2,4-dinitrochlorobenzene-2,4-dinitrophenol.
e) Benzoin-benzil-benzilic acid.
f) Acetanilide-p-bromoacetanilide-p-bromo aniline.

4. Use of Computer (ChemDraw, ChemSketch, ISI Draw):

Draw the structure of aliphatic, aromatic and heterocyclic compounds and get the correct IUPAC name.

Reference Book:

1. Vogel practical organic chemistry.

M. Sc. I Semester
Laboratory Course III
Paper : VI1 (CH - 417) (Physical Chemistry)

Marks: 50 **132P**

N.B. 1. Performance of eighteen experiments is expected
2. At least one experiment on each instrument should be done.
3. Student should prepare the required solutions

SECTION-A:
INSTRUMENTATION:

1. CONDUCTOMETER:

1. To estimate the concentrations of sulphuric acid, acetic acid and copper sulphate in given solution.
2. To determine solubility product and thermodynamic properties (ΔG , ΔH, ΔS) of sparingly soluble salts.
3. To determine the relative strength of chloroacetic acid and acetic acid.
4. To determine the hydrolysis constant of Aniline hydrochloride.
5. To investigate basic hydrolysis of ethyl acetate at four different temperatures and to find out the energy of activation .

2. POTENTIOMETER:

1. To determine PK_1 PK_2 values of Phosphoric acid.
2. To determine strength of strong acid and weak acid in given mixture.
3. To determine the oxidation state of metal ion by method of concentration cell without transparence.

3. pH-METER:

1. To determine Hammet constant of given substituted benzoic acid.
2. To determine pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence to find out dissociation constant of acid.

4. COLORIMETER

1. To determine equilibrium quotient for formation of mono thiocyanate iron(III) complex.
2. To determine Indicator constant of an indicator.
3. To determine concentration of Cu(II) iron in given solution titrating with E.D.T.A. solution.

5. REFRACTOMETER:

To determine the molar refractivity of methyl acetate, ethyl acetate,

n-hexane and carbon tetra chloride and to calculate refractive equivalence of C, H and Cl atom.

2. To study the variation of refractive index with composition of mixture of CCl_4 and ethyl acetate.

6. POLARIMETER.

1. To determine the relative strength of two acids.
2. To determine the percentage of two optically active substance (d-glucose and d-tartaric acid) in the mixture.

SECTION B
NON-INSTRUMENTATION

1. To determine partial molar volume of ethanol and water mixture at given Composition .
2. To determine molecular weight of high polymer by viscosity measurement.
3. To study the effect of surfactant on surface tension of water by using stalagmometer.
4. To determine solubility of benzoic acid at different temperature and hence to determine it's heat of solution.
5. To investigate the autocatalytic reaction between $KMnO_4$ and oxalic acid and to find energy of activation.
6. To determine the rate constant of hydrolysis of methyl acetate catalyzed by HCl.
7. To determine effect of ionic strength on rate constant of reaction between potassium per sulphate and potassium iodide.
8. To investigate the solubility of three component system and hence tie line on binodal curve.
9. To study the variation of viscosity with composition of mixture of i)ethanol-water ii) methanol-ethylidene chloride iii) nitric acid- Chloroform and determine whether or not there is compound formation between two liquids.
10. To determine surface tension of methyl acetate, ethyl acetate and chloroform and hence to calculate atomic parachors of C, H, Cl.
11. To determine order of reaction of given reaction kinetics by fractional change method.
12. To study distribution of benzoic acid between benzene and water at room temperature and hence show that benzoic acid dimerises in benzene.

M. Sc. I Semester
Laboratory Course IV
Paper : V111(CH - 418) (Analytical Chemistry)

Marks: 50 **132P**

Section-A
(Intrumental)

1. Conductometry

1. Determination of the strength of strong acid and weak acid from mixture solution conductometrically
2. Analysis of aspirin by conductometric method.

2. Potentiometry

1. Determination of the strength of halides in the given mixture using Potentiometry.
2. Determine the acid and basic dissociation constant of an amino acid (Glycine) and hence isoelectric point of an acid

3. pH-metry

1. Acid-base titration in non-aqueous media by pH-metry (benzoic acid in ethanol / NaOH).
2. Determination pKa of weak acid by pH-metry.
3. Determination of degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

4. Colorimetry

1. Varification of Beer's law for a) $KMnO_4$ and Cu^{+2} ammonia complex solution.
2. Determination of empirical formula for the formation of ferric salicylate complex by Job's method.
3. Determination of stability constant for the formation of complex between Fe^{+3} ions and 5-sulphosalicylic acid.

5. Polarimetry

1. Determination of rate constant for inversion of cane sugar by polarimetry.
2. Study of inversion of cane sugar by enzyme kinetics.
3. determine the percentage of two optically active substances in a mixture polarimetrically.

6. Flame photometry

1. Estimation of Na^+ / K^+ by Flame photometry.

Section-B
(Non-Instrumental)

1. Statistical analysis

1. Application of 't' test for experimental data.
2. Application of rejection criteria ('Q' test) for experimental data.
3. Treatment of analytical data with least square method applied to Beer's law for $KMnO_4$ solutions.

2. Chromatography

1. Separation of cations and anions by paper chromatography and determination of Rf values.
2. Determination of Ion-exchange capacity of an cation exchanger.
3. Determination of Ion-exchange capacity of an anion exchanger.

3. Chemical Kinetics

1. Investigate the reaction between bromic acid and hydroiodic acid.
2. To study the kinetics of iodination of acetone.

4. Heterogeneous equilibria:

1. Determine the formula of complex form between Cupric ion and ammonia by distribution method.
2. Investigate the solubility of three component system and hence draw a tie lone on bimodal curve.
3. Determination of hardness of water by complexometric titration.