# KARNATAK UNIVERSITY, DHARWAD

*Post-graduate Department of Chemistry*

## SYLLABUS FOR M.Sc. CHEMISTRY

(With effect from 2004 onwards)

### SEMESTER – I

### CHI-1.1: INORGANIC CHEMISTRY

Structure, Bonding and Coordination Chemistry

Review of periodicity of properties: Atomic size, ionic radii, ionization potential, electron affinity, and electronegativity, applications of electronegativity. Fundamental trends, first and second row anomalies, diagonal relationships, periodic anomalies of the non-metals and post-transition metals. 6 hrs.

Ionic bonding: Properties of ionic compounds, lattice energy, Born-Lande's equation, Born-Haber cycle and its applications, Kapustinskii equation, Solvation energy, dissolution of ionic compounds in polar solvents and its energetics. The predictive power of thermochemical calculations of ionic compounds, covalent character in ionic compounds. Radius ratio and structure of ionic compounds, efficiency of packing of crystal lattices. 5 hrs.

Covalent bonding:Valence bond theory, orbital overlap. Molecular orbital theory, symmetry and overlap, molecular orbital diagrams of diatomic molecules (homo- and hetero- nuclear), triatomic molecules, linear ($CO_2$ , $N_2O$ ) and angular ($NO_2$), Walsh diagrams, Bent's rules, some reactions of covalently bonded molecules, Resonance, hybridisation, VSEPR theory, molecular geometries. 5 hrs.

Hydrogen bonding: Types, detection and theories
1 hrs.

Metallic bonding: Characterization of metallic states, VB approach, band theory, conductors, insulators, semiconductors, defects in solids.

3 hrs.

Stereochemistry of coordination compounds: coordination geometry, types of isomerism (geometrical & optical)

Bonding in coordination compounds: crystal field theory (CFT) of coordination compounds, splitting of d-orbitals in octahedral, tetrahedral and square planar complexes, CFSE, factors affecting the magnitude of 10 Dq, measurement of 10 Dq, Spectrochemical series, short comings of CFT, Jahn-Teller distortion in coordination compounds. Molecular orbital theory applied to coordination compounds without pi-bonding. 9 hrs.

Magnetism, Types, Spin moment, spin-orbit coupling, introduction to absorption spectra of coordination compounds (d systems only).

3hrs.

Metal-ligand equilibria: Stepwise and overall formation constants, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of formation constants by polarography and spectrophotometry.

5 hrs.

Organometallic chemistry: Classification of organo-transition metal complexes, The 18-electron and 16-electron rules. Synthesis, structure, bonding and reactions of metal alkyls, aryls and olefin complexes. 5 hrs.

Metal clusters: Halide clusters, compounds with metal-metal multiple bonds. 2 hrs.

Metal -complexes: Preparation, structure, bonding and important reactions of metal carbonyls, metal nitrosyls, dinitrogen and dioxygen complexes.

3 hrs.

Concepts of Acids and Bases: Bronsted and Lewis acids and bases, pH and $pK_a$, acid-base concept in non-aqueous media, HSAB concept, buffers.

3 hrs

Total 50 hrs

*Books Recommended:*


1. Inorganic Chemistry, 4$^{th}$Edn. J. E. Huheey, E.A. Keiter and R. S. Keiter. Addission-Wesley ( 1993 ).
2. Inorganic Chemistry, 2$^{nd}$Edn. ( ELBS ), D.F.Shriver, P.W.Atkins and C.H.Langford. Oxford University Press (1994 )
3. Basic Inorganic Chemistry, 3$^{rd}$Edn. F.A.Cotton, G.Wilkinson and P.L.Gaus, John-Wiley and sons (1995 )
4. Concepts and models in Inorganic chemistry 3$^{rd}$Edn. B.Douglas. D.H.Daniel and J.J.Alexander, John-Wiley and Sons (1983).
5. Concise Inorganic chemistry- J.D.Lee, 5$^{th}$ Edn, New Age International (1996).
6. Inorganic chemistry- K.F.Purcell and J.C.Kotz (W.B.Saunders san Francisco ).


CHO-1.2: ORGANIC CHEMISTRY

Reaction Mechanism, Stereochemistry, Heterocycles and Natural products.

Bonding and Aromaticity:

*Bonding in Organic Molecules :* Atomic and molecular orbitals. Concept of bonding, localized chemical bonding, antibonding and nonbonding molecular orbitals. Hybridisation, geometry and shape of simple molecules. Bond order, bond angle, bond length and bond energies.

*Structure and reactivity :* Concept of organic acids and bases. Electronic and steric effects on acidity and basicity.

*Aromaticity :* Aromaticity and Huckel's rule. Benzenoid and non-benzenoid aromatic compounds. Alternant and non-alternant hydrocarbons. Aromaticity of charged ring systems ( three to eight membered), tropone, azulene and ferrocene. Non-aromatic and anti aromatic systems.

10 hrs

Reaction mechanism:

*Organic reaction mechanism :* Classification of reactions, meaning and importance of reaction mechanism. Kinetics. Mechanism of nucleophilic substitution reactions. Variables in $S_N1$, $S_N2$ and $S_Ni$ reactions.

*Reactive intermediates :* Formation, stability and some important reactions of carbocations, carbanions and free radicals. 10 hrs

Stereochemistry:

Elements of symmetry and symmetry operations. Optical isomerism. Cahn-Ingold-Prelog nomenclature. Geometrical isomerism.

E-,Z- nomenclature. Methods of determining configuration of geometrical isomers. Projection formulae : Fischer, perspective,Sawhorse and Newman projection formulae and their interconversions. Optical isomerism due to one or more chiral centres. Enantiomers, diastereomers and epimers. Psuedoasymmetric compounds. Racemisation and resolution. 10 hrs.

Chemistry of heterocyclic compounds :

Nomenclature, structure, reactivity, synthesis and chemical reactions of the following heterocycles:

Pyrazole, Imidazole, Oxazole, Isoxazole, Thiazole, Indole and Benzimidazole. 10 hrs.

Chemistry of natural products :General methods of structure elucidation of alkaloids and terpenoids. Alkaloids : Structure elucidation and synthesis of Atropine, Cinchonine Quinine and Papaverine.

*Terpenoids :* Structure elucidation and synthesis of Pinene, Camphor, Zingiberene and Farnesol.

10 hrs.

Total 50 hrs.

*Books Recommended :*


1. Organic Chemistry- by R. T. Morrison and R. N. Boyd, 5th Edition, Allyn and Bacon New Delhi.
2. Organic Chemistry – by C. H. Heathcock and Streitweiser, Collier- McMillan, New York (1979).
3. Basic Principles of Organic Chemistry- by J. D. Roberts and M. C. Caserio.
4. Organic Chemistry- Vol. I & II by I.L.Finar 6th Edition. 1998. ELBS, London
5. Stereochemistry – by G. R. Chatwal
6. Stereochemistry – Conformation and Mechanism by P. S. Kalsi, Wiley – Eastern Ltd, New Delhi (1992).
7. Stereochemistry of Carbon Compounds – by E. L. Elied Tata Mc Graw Hill, New Delhi (1976).
8. Organic Stereochemistry – by H. Kagan, Edward Arnold (1979).
9. Guide Book to Mechanism in Organic Chemistry – by Peter Sykes.
10. Organic Chemistry Vols. I-III by S. M. Mukherji, S. P. Singh and R..P. Kapoor, Wiley Eastern (1992).
11. Advanced Organic Chemistry, Reactions, Mechanism and
12. Mechanism and Theory in Organic Chemistry – by E. S. Gould.
13. Heterocyclic Chemistry – by J. A. Joule and G. F. Smith, 2nd Edition, Van Nostrand (London) 1978.

14. Heterocyclic Chemistry – by T. L. Gilchrist, Butterworths (London) 1985.

15. Introduction to the Chemistry of Heterocyclic Compounds – by R. M. Acheson.

16. The Alkaloids, Vol I. By K. W. Bentley, Interscience (London).

CHP-1.3: PHYSICAL CHEMISTRY-I

1. Quantum Chemistry:

Black body radiation, Planck's theory, Photoelectric effect, Compton effect. Bohr theory of hydrogen atom, Sommerfeld theory.

Wave- particle duality: de Broglie hypothesis, uncertainty principle, the wave nature of electron. 7hrs

Schrodinger equation. Wave function and its interpretation. Normalization and orthogonality, eigen functions and eigen values. 3 hrs

Solutions of equations of a free particle, particle in a box Problem: in one and three dimensions. Rigid rotator and the harmonic oscillator. Equation for the hydrogen atom in spherical polar coordinates and an indication of the method of its solution, the quantum numbers and their significance. 8 hrs

Hydrogen-like atoms, properties of the H-atom wave functions. Electronic energy states of H-atom. Many electron systems and the self consistent field method. Electronic configurations in the periodic table. Pauli exclusion principle. Spectroscopic term symbols. 6hrs

1. Reaction Kinetics: Kinetics and Mechanism: Steady state approximation and simple examples relating kinetics to mechanism.
2 hrs

Kinetics in solution: Primary and secondary salt effects. Effect of solvent.
2 hrs

Chain Reactions: examples of chain reactions, general aspects of chain reactions. Chain-length, Chain transfer reactions, Chain inhibition, Kinetics of branching chain reactions, explosion limits. 4 hrs

Mechanism of heterogeneous catalysis. BET theory, Gibbs adsorption equation. 3 hrs

A critical account of collision and transition state thories.

Theories of unimolecualr reactions: RRKM theory. Isomerisation of methyl isocyanide. 4 hrs

Flash photolysis and applications. Chemiluminescence. 1hrs

3. Thermodynamics

Thermodynamic criteria for spontaneous chemical changes. Standard free energies and their determination.

Relation between free energy change and equilibrium constant.

The pressure dependence of free energy of non-ideal gases; fugacity. Standard state for non-ideal gas. Equilibrium constants in non-ideal systems. Temperature dependence of free energy and equilibrium constants.
10 hrs

Total: 50hrs

*Books Recommended:*

1Introduction to Quantum Chemistry by A. K. Chandra, Ed. 3, Tata McGraw Hill, New Delhi, 1988.

2.Quantum Chemistry by R. K. Prasad, New Age International Publications, New Delhi, 1997.

3.Quantum Chemistry by Eyring, Walter and Kimball, John-Wiley, New York.

4.Physical Chemistry by G. M. Barrow, McGraw Hill, New York, 1996.

5.Fundamentals of Physical Chemistry by Maron and Lando.

6.Physical Chemistry by P. W. Atkins, ELBS, London, 1990 (Ed. 4).

7. Physical Chemistry by K. Vamulapalli, Prentice Hall of India Pvt. Ltd., New Delhi, 1997.

8.Physical Chemistry by Daniels and Alberty, Wiley, New York.

9. Physical Chemistry Through Problems by S. K. Dogra and SDogra, Wiley Eastern, New Delhi.

10. A Text Book of Physical Chemistry by Samuel Glasstone, McMillan, London.

11. Atomic Structure and Chemical Bonding by Manas Chanda, Tata McGraw Hill Publishing Co., New Delhi.

12. Chemical Kinetics by K. J. Laidler, Tata McGraw Hill Publishing Co., New Delhi.

13. 13.Kinetics and Reaction Mechanisms by Frost and Pearson, Wiley, New York.

14.Thermodynamics for Chemists by S. Glasstone, Van Nostrand, Princeton.

15. Thermodynamics by Rajaram and Kuriocose.

16.Fundamentals of photochemistry by K.K Rohtagi-Mukherjee, Wiley Eastern, New Delhi.

CHI (Pr) 1.4: LAB. COURSE IN INORGANIC CHEMISTRY

*a) Quantitative analysis*

Separation and determination of two metal ions involving volumetric and gravimetric methods from the following

a) Fe + Ni, Cu + Fe, Cu + Ni and Ni + Zn.

b)Computer applications

c)Paper Chromatography

Scheme of Examination

a) Separation and estimation of two ions

One volumetrically, the other by gravimetric method

| | |
|---|---|
| i). Volumetric | 35 |
| ii). Gravimetric | 35 |
| iii). Viva | 05 |
| iv). Class records | 05 |

Books Recommended

1.Vogel's Text Book of Quantitative Inorganic Analysis, J. Basett, R.C.Denney, H.Jeffery and J.Mendham, Longmans, Green and company Ltd.

CHO (Pr) 1.5: LAB. COURSE IN ORGANIC CHEMISTRY

Experiment No. 1:

Preparation of the following Organic compounds

1) Benzoic acid and Benzyl alcohol from benzaldehyde (Cannizarro reaction )
2) p-Bromoaniline from acetanilide.
3) p-Nitroaniline from acetanilide.
4) p- Chlorobenzoic acid from p- toluidine.
5) Aniline from Benzene.
6) 2,4,-Dinitrophenol from Chlorobenzene.
7) Benzil from Benzaldehyde.
8) m-Nitroaniline from Nitrobenzene.
9) Methyl orange.
10) m-Nitro benzoic acid from Ethyl benzoate.
11) Benzanilide from Benzophenone (Beckmann rearrangement).
12) 2-Hydroxy-5-methyl benzophenone from p-cresol (Fries rearrangement).

Experiment No. 2.

Estimations:

1. Estimation of acid and amide in a given mixture.
2. Estimation of acid and ester in a given mixture.
3. Determination of molecular weight of a Base by hydrochloride method.

Scheme of Examination

Experiment No. 1—-Preparation—40 marks

Experiment No. 2—-Estimation —30 marks

Journal & viva—10 marks

CHP (Pr)-1.6: LAB. COURSE IN PHYSICAL CHEMISTRY.

I. Calibration

Calibration of glassware and weight box

II. Density:

Determination of partial molar volume (eg.. Salts in water and liquids in water, systems)

III.Viscosity:

Molecular radius of glycerol molecule and molecular weight of a polymer by viscosity measurements

IV. Distrubution law:

Distribution of benzoic acid (or succenic acid, etc.) between water and benzene.

V. Thermochemistry:

i) Step -wise heat of neutralization of a polybasic acid

ii) Integral heats of solution and heats of dilution of salts. (e.g., $KNO_3$, NaCl etc.)

VI. Refractometry:

Molar refraction of a solid substance by measuring the refractive indices of its solutions.

VII. Spectrophotometry:

i) Mixture analysis by absorptiometry/Spectrophotometry.

ii) Applicability range (for an absorbing substance in solution) and evaluation of the molar absorbancy index, finding unknown concentration.

VIII. Reaction Kinetics:

Acid hydrolysis, catalytic strengths and determination.of $E_a$.

IX. Potentiometery:

Dissociation constant of weak monobasic acids and titration of $HCl+CH_3COOH$ with NaOH.

X. Electrical conductance:

i. Titration of a weak acid with a weak base and a strong acid with a weak base.

i. Titration of acid mixture with NaOH.

e.g. $CH_3COOH$ + HCl; $CH_3COOH$ + $H_2C_2O_4$;

$HNO_3$ + $H_2SO_4$; $H_2C_2O_4$ + HCl

*Books Recommended:*


1. Practical Physical Chemistry by A. M. James and F. E. Prichard, Longmans, London.
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill, New York.
3. Experiments in Physical Chemistry by Daniels, Alberty and Willams, McGraw Hill, New York.
4. Experimantal Physical Chemistry by W. G. Palmer, Cabridge University Press, London.
5. Advanced Physico-Chemical experiments by J. Rose.
6. Text Book of Physical Chemistry by S. Glasstone, , McGraw Hill,London.
7. Text book of Quantitative Analysis by A. I. Vogel, ELBS, Harlow.
8. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publishing House.
9. Experimental Physical Chemistry by V. D. Athawale and Parul Mathur, New Age International Publishers.


Scheme of Examination:

1) Experiment –I ———————— 35 marks
2) Experiment-II ———————— 35 marks
3) Journal ———————— 05 marks

4) Viva Vice ———————— 05marks

SEMESTER –II

CHI-2.1: INORGANIC CHEMISTRY

Chemistry of Non-transition elements, Separation Techniques and Group Theory

Chemistry of non-transition elements

General discussion on the properties of the non-transition elements, special features of the elements B, C, Si, N, P, O, S, and F

Syntheses, properties and structure of Boranes, Borazines, Silicates, phosphazenes, S-N compounds, Silicones, Carboranes, Peroxo compounds of boron, carbon and sulphur. Oxyacids of nitrogen, phosphorus, sulphur and halogens. 12 hrs.

Interhalogen compounds and pseudohalogens. 2 hrs.

Noble gas compounds: Preparation and structure of noble gas compounds (oxides, fluorides). 3 hrs.

Separation techniques

*Ion exchange:*

Types of ion exchange resins, ion exchange capacity, ion exchange equilibria and selectivity coefficient. Techniques, ion exchange process.

Applications of ion exchangers: Preparation and purification of reagents, removal of interfering ions, concentration and recovery of traces, determination of total salts (stoichiometric substitution) and in the separation of Lanthanides and Actinides.

5 hrs.

*Solvent extraction:*

Basic principles of solvent extraction, relationship between percentage extraction and distribution ratio and distribution selectivity of an extraction. Techniques of extraction and choice of solvents, stripping, back washing, treatment of emulsion, variation of oxidation states, use of masking out and salting out agents. Classification of solvent extraction methods. Synergistic extractions. Applications of solvent extraction.

5 hrs.

*Chromatography:*

General principles and classification of chromatographic methods: Paper, Thin-layer, column and liquid chromatography.

Gas chromatography : Principles, instrumentation, stationary phases and types of carrier gas used in GC. Methods of sample injection, types of detectors used, programmed temperature GC, plate and plate height in GC. Applications of GC, use of GC-MS in detection of samples. HPLC and its applications.

7 hrs.

Symmetry and Group theory

Molecular symmetry, Representation of symmetry operation as matrices. Definition of groups, set of symmetry operations of molecules satisfying the condition of point groups. Representation, basis of representation, reducible and irreducible representation. The great orthogonality theorem, character tables and their applications to chemical bonding. 10 hrs.

Data analysis

Errors: Types of errors, propagation of errors, accuracy and precision, Standard deviation least square analysis, and significant figures.

6 hrs.

Total 50 hrs.

*Books Recommended*


1.Inorganic Chemistry, 4th Edn. J. E. Huheey, E.A. Keiter and R. S. Keiter. Addission- Wesley (1993)

2.Comprehensive Inorganic Chemistry, Ed., J.C.Bailar, H.J.Emeleus, R.S.Nyholm and A.F.Trotman.

3.Advanced Inorganic Chemistry, 3rd & 5th Edn., F.A.Cotton and G. Wilkinson, John-Wiley and sons.

4.Analytical Chemistry, 5th Edn, G.D.Christian, John- Wiley and Sons Inc.(1994).

5. Fundamentals of Analytical Chemistry, 7th Edn, D.A.Skoog. D.M.West and F.J.Holler, Saunder College Publishing ( 1996 ).

6. Instrumental Methods of Analysis, H.H.Willard, L.L.Merrit. J.A.Dean and F.A.Settle, CBS Publishers (1996).

7. Chemical Applications of Group Theory 2nd Edn, F.A.Cotton, Wiley Eastern Ltd (1976).

8. Symmetry and Spectroscopy of Molecules, K. VeeraReddy New Age International, (1998).

9. Group Theory for Chemists, G.Davidson Macmillan, (1991).

10. Vogel's Text Book of Quantitative Inorganic Analysis, J. Bassett, R.C.Denney, G.H.Jeffery and J.Mendham, Longman Green and company Ltd.


CHO 2.2: ORGANIC CHEMISTRY

Reaction mechanism, Stereochemistry, Heterocycles and Natural products - II

Advanced stereochemistry

Prochirality: Homotopic, enantiotopic, diastereotopic groups and faces. Optical isomerism due to molecular dissymmetry -allenes, spiranes and biphenyls.

Conformational analysis: Ethylenechlorohydrin, 1,2-dichloroethane, 2-aminoethanol, cyclobutane, cyclohexane. Conformation and reactivity of monosubstituted cyclohexanes. Curtin-Hammet principle. 10 hrs

Reaction mechanism - II

Mechanism of aromatic substitution reactions—Electrophilic, Nucleophilic and Benzyne pathways. Product proportions in aromatic electrophilic substitution reactions and Hammonds postulate .

*Named Reactions:*

Aldol, Stobbe, Dieckmann, Reimer-Tiemann, Reformatsky, Diels-Alder reaction, Wittig reaction, Robinson annelation, Michael addition, Mannich reaction.

10 hrs

Chemistry of Heterocyclic Compounds -II

Nomenclature, Structure, reactivity, synthesis and chemical reactions of Pyrimidines, Purines, Quinoline, Isoquinoline..

Oxygen Heterocycles: Coumarins and chromones,

Flavones: Flavone and 7-hydroxy flavone.

Isoflavones: Isoflavone and Daidzein. Crown Ethers: Chemistry and applications of [18]-Crown-6-ether.

10 hrs

Natural products - II

Chemistry of Vitamins $B_1$, $B_2$, $B_6$.

Proteins and Peptides: primary-structure of Peptides and Proteins (end group analysis).

Description of secondary, tertiary and quaternary structures.

Synthesis of Peptides: Protecting groups in peptide synthesis, structure and synthesis of Glutathione. Solid- phase Peptide synthesis.

10 hrs

Carbohydrates

Oxidation methods to determine the ring size of Glucose. Derivatives of Monosaccharides-Acetone sugars, Aminosugars and Deoxysugars. Conformation of Glucose and anomeric effect.

Disaccharides: Structure elucidation of Maltose and Sucrose

Polysaccharides: Structure of starch and cellulose.

10 hrs

Total 50 hrs

*Books Recommended*


1. Stereochemistry of Carbon Compounds – by E. Eliel, McGraw Hill.
2. Organic stereochemistry - by Henri Kagan, Edward Arnold, 1979.
3. Organic Stereohemistry – by G. Hallas, McGraw Hill, 1967.
4. Stereochemistry – by V. M. Potapov, Mir Publishers (Mascow) 1979.
5. Stereochemistry of Organic Compounds, Principles and Applications by D. Nasipuri, Wiley Eastern Ltd, 1992.
6. Stereochemistry : Conformation and Mechanism by P. S. Kalsi- Wiley Eastern Ltd, 1992.
7. Mechanism and Theory in Organic Chemistry by E. S. Gould, Holt, Rinhert and Winston.
8. Advanced Organic Chemistry, Reaction, Mechanism and Structure by Jerry March, 3rd Edition Wiley Eastern Ltd.
9. Organic Reaction Mechanism by Harris and Wasmer, John Wiley.
10. Advanced Organic Chemistry : Structure and Mechanism – by Francis A. Carey and Rechard J. Sundberg. Plenum Press. New York and London (Part I and Part II Reactions and synthesis 1977).

11. Organic Chemistry by Mukherji S. M, Singh. S. P, and Kapoor. R. P. Vol. I, II and III Wiley Eastern Ltd.
12. Organic Reaction Intermediates, Edited by McMannus. Academic Press
13. Reactive Intermediates in Organic Chemistry by Issac. John – Wiley.
14. Organic Chemistry, by R. T.Morrison and R. N. Boyd (Allyn and Beaon, Inc, Universial Book Stall) Boston, London, Sydney, New Delhi.
15. Organic Chemistry, by T. W. Grahmons, John Wiley & sons.
16. Chemistry ofVitamins by S. F. Dyke, Interscience London 1965.
17. Organic Chemistry by I. L. Finar, 6th Edition ELBS London 1998.
18. Peptides and Proteins by T. D. Elmore.
19. Chemistry of Carbohydrates by G. C. Percival.
20. Carbohydrates – Chemistry and Biochemistry by Pigman and Harton.

CHP-2.3: PHYSICAL CHEMISTRY-II

1. Molecular Spectroscopy:

Electromagnetic radiation and its interaction with matter. Atomic and molecular spectra. Rotational spectra of a rigid and non-rigid planar simple molecules. Vibrational spectra of harmonically vibrating diatomic molecules, anharmonic case. Morse potential function and dissociation energy. The diatomic vibrating rotator; the vibrations of polyatomic molecules, specific group vibrations. Applications of infrared spectroscopy.

Raman spectra: Raman effect, Rotational Raman and vibrational Raman spectra of simple molecules.

Electronic spectroscopy of diatomic molecules. Born-Oppenheimer approximation. Vibrational course structure of electronic transitions: The $v'$ and $v''$ progressions. Deslandres table. Intensity: the Franck-Condon principle. Predissociation.

15 hrs

2.Diffraction studies:

Crystallography: Crysatl habit, symmetry elements, Miller indices, X-ray diffraction, Laue method, Bragg's law. The Rotating crystal method, Powder method. Structure factor and determination of the crystal structure.
8 hrs

3. Thermodynamics:

A review of the thermodynamics of ideal solutions. Non-ideal liquid systems. Partial miscibility. Activity and activity coefficients of components of solutions, partial molar quantities and their determinations. Gibbs-Duhem equation and the calculation of activity of a component in solutions. Duhem-Margules equation. Ternary systems: phase diagram of ternary systems. 7 hrs

4. Electrochemistry:

Debye-Huckel theory of activity coefficients, Debye-Huckel limiting law and Debye-Huckel-Onsagar theory of conductance of strong electrolytes.

5 hrs

5. Computer Applications:

Basic structure of the computer, functioning of the computer, memory, I/O device, secondary storages.

Operating systems: DOS, WINDOWS, UNIX and WORD

Introduction to selected packages

MATALAB, FOXPRO, EXCEL

Computer programming in basic, Fortran, C 15 hrs

Total: 50 hrs

*Books Recommended:*


1. Fundamentals of Molecular Spectroscopy by C. N. Banwell, Tata McGraw Hill Publishing Co., New Delhi.
2. An introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill, New York.
3. Molecualr Spectra and Molecular Structure:I Spectra of Diatomic Molecules by G. Herzberg, Van Nostrand, Princeton.
4. Physical Chemistry By P. W. Atkins, ELBS, London.
5. Physical Chemistry by G. M. Barrow, McGraw Hill, New York.
6. Atomic and Molecular Spectroscopy by M. C. Gupta, New AgeInternational Publishers, New Delhi.
7. X-ray Crystallography by Buerger, Wiley, New York.
8. X-ray Diffraction by D. B. Cullity, Addison Wesley. Massachusetts.
9. Thermodynamics for Chemists by S. Glasstone, Van Nostrand, Princeton.
10. Thermodynamics by Rajaram and Kuriocose.
11. An Introduction to Electrochemistry by S. Glasstone, Van Nostrand, London.
12. A Text Book of Electrochemistry by G. F. A. Kortum and J. O. M. Bockris, Elsevier, New York.
13. Modern Electrochemistr by J. O. M. Bockris and A. K. N. Reddy. Vol-I and Vol-II, Butterworths, London.
14. Computational chemistry by A. C. Norris, John Wiley.
15. Computer Programming in FORTRAN 77 by R. Rajaraman, Pretice Hall.
16. Numerical Analysis, by C. E. Forgberg, MacMillan.
17. Numerical Analysis- A Practical Approach, by M. J. Maron, John Wiley.
18. Numerical Methods for Scientists and Engineers, by H. M. Anita, Tata McGraw Hill.
19. Programming with Ansi C, by Balaguruswamy.


CHI (Pr) 2.4: LAB. COURSE IN INORGANIC CHEMISTRY

a) Semimicro qualitative inorganic analysis of a mixture. Mixture containing 3 cations and 3 anions including one less common cation such as Mo, Ti, Zr, V and Li and interefering anions.

b) Preparation of Complexes

c)Volumetric exercise without involving separation. Eg: $MnO_2$ in Pyrolusite.

*Books Recommended:*


1.Chemical Semimicro analysis, V.N.Alexeyev, Mir Publishers, Mascow (1975).

2.Vogel's Qualitative Inorganic Analysis. Revised by G.Svehla, Longmann Group Ltd (1998).

3.Practical Inorganic Chemistry, G.Pass and H.Sutcliff, Chapman and Hall Ltd.(1968).

4. Vogel's Text Book of Quantitative Inorganic analysis, J.Basett, R.C.Denney, G.H.Jeffery and .Mendham, Longmans, Green and Company Ltd.

Scheme of Examination

| | |
|---|---|
| a) Qualitative analysis | 50 |
| b) Volumetric exercise / Preparation of a complex | 20 |
| c) Viva | 05 |
| d) Records | 05 |

CHO (Pr) 2.5: LAB. COURSE IN ORGANIC CHEMISTRY

Experiment No. 1: Qualitative analysis of a Binary mixture.

Experiment No. 2: Preparation of two Derivatives.

Scheme of Examination

| | |
|---|---|
| Experiment No. 1 | |
| Qualitative analysis | 50 marks |
| Experiment No.2 | |
| Prep$^{n}$ of derivatives | 20 marks |
| Journal & viva | 10 marks |

*Books Recommended*

1) Vogel's Text Book of Practical Organic Chemistry- by B.S.Fumiss, AJ Hannaford, P.W.G.Smith and A. Tatchel, 5th edition 1997, ELBS Longman, London.
2) Experimental Organic Chemistry-by L.M.Harword & C.J.Moody. Blackwell, Oxford London First edition.

CHP(Pr)-2.6: LAB. COURSE IN PHYSICAL CHEMISTRY

I. Surface Tension:

Variation of surface tension of aqueous solutions of n-propyl alcohol with concentration and determination of the limiting cross sectional area of the molecule.

Effect of added salt on surface tension of water (and/or comparison of the cleansing powers of the two detergent samples).

II. Solubility:

Heat of solution of an organic compound by solubility experiments and the effect of addition of an electrolyte on the solubility.

III. Phase Equilibria:

Equilibrium constant of the reaction : $KI + I_2 \quad KI_3$

IV. Thermochemistry:

Heat of neutralization of a weak acid and calculation of its heat of ionization.

V. Spectrophotometry:

Investigation of complex formation. (eg. $Fe^{+3}$ + Salicyclic acid system: formula, stability, G value calculation and pH effects).

VI. Electric conductance:

i. Equivalent conductance of a weak electrolyte at different concentrations and the applicability of Ostwald's law.

ii. Verification of the Onsagar equation for strong electrolytes.

iii. Equivalent conductance of a weak electrolyte from Kohlrausch's law.

VII. Reaction kinetics:

a. Salt effect on the persulphate-iodide reaction.

b. Iodination of acetone.

c. Autocatalysis: Mn(VII)-Oxalic acid case in the presence of $H_2SO_4$.

VIII. EMF of cells:

a. Solubility of sparingly soluble salts.

b. Titration of $Fe^{2+}$ with $Ce^{4+}$ (or $Cr^{6+}$) and determination of the formal redox potentials of the couplexes of $Fe^{3+}/Fe^{2+}$ and $Ce^{4+}/Ce^{3+}$ (or $Cr^{6+}/Cr^{3+}$).

c. Titration of Zn(II) with $Fe(CN)_6^{4-}$ and determination of the empirical formula of the complex formed.

IX. Cryoscopy:

i. Determination of the degree of dissociation of a given strong electrolyte and the determination of the number of ions present in the solute.

ii. Determination of the molecular weight of the given solute by the vacuum flask method.

*Books Recommended:*

1.Findlay's Practical Physical Chemistry, 9th edition, revised by B. P. Levitt, Longman, London.

2.Practical Physical Chemistry by A. M. James and F. E. Prichard, Longman, London.

3.Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill New York.

4. Experiments in Physical Chemistry by Daniels, Alberty and Willams et al, McGraw Hill New York.

5.Laboratory Physical Chemistry by Oelke/M.A.C.T.L.A.C.

6. Experimental Physical Chemistry by W. G. Palmer, C.U.P., London.

7.Advanced Physico-Chemical experiments by J. Rose.

8.Text book of Physical Chemistry by S. Glasstone, Macmillon and Co., London.

9.Text book of Quantitative Analysis by A. I. Vogel, ELBS, Harlow.

10.Advanced Practical Physical Chemistry by J. B. Yadav. Goel Publishing House.

11.Experimental Physical Chemistry by V. D. Athawale and Parul Mathur, New Age International Publishers.

Scheme of Examination

1)Experiment –I ———————— 35 marks

2) Experiment-II ———————— 35 marks

3) Journal ———————— 05 marks

4) Viva Vice ———————— - 05marks

SEMESTER - III

INORGANIC CHEMISTRY

CHI-3.1 ; Advanced Coordination Chemistry and Bioinorganic Chemistry

Review of theories, Molecular orbital theory/Ligand field theory (octahedral, tetrahedral and square planar complexes), Evidences for metal-ligand orbital overlap.

4-hrs.

Electronic spectra : Spectroscopic ground terms, correlation diagrams, selection rules, Orgel and Tanabe-Sugano diagrams for

transition metal complexes ($d^1$-$d^9$ states), Racah parameters, interpretation of spectra of 3d metal ions, spin-orbit and vibronic effects, charge transfer spectra.

5 hrs.

Magnetic properties : Types of magnetic behaviour, diamagnetic contributions, TIP, orbital contribution, quenching of orbital-angular moment, Spin-orbit coupling,ferro-,ferri-and antiferro magnetism, spincrossover in co ordination compounds, Gouy and Farady techinques. 5 hrs.

Stereoisomerism : Chirality,optical activity, CD, ORD, Cotton effect and magnetic circular dichroism, absolute configurations. 3 hrs.

Reaction mechanism of coordination compounds : Energy profile of a reaction, inter and labile complexes, Electron transfer reactions, Marcus theory, mechanism of electiron transfer reactions outer sphere and inner sphere electrion transfer reactions, complimentary and non-complimentary reactions. Synthesis using electron transfer reactions.

Classification of ligand substitution mechanism, substitution in octahedral complexes, Acid hydrolysis, Base hydrolysis, substitution reactions in square planar complexes, trans effect. 8 hrs.

Photochemistry of Coordination compounds :

Electronically excited states of metal complexes, Types of photochemical reactions, photochemistry of metallocenes, Ruthenium and chromium complexes.

3 hrs.

Bioinorganic Chemistry

Membranes and cation transport :

Cell, significance of ionophores,Ion transport (Na,K,Ca,Mg,) in biological systems.

Metalions and chelating agents in biology and medicine :

Metal, metal complexes as therapeutic agents treatment of toxicity due to inorganics (chelation therapy). Metal ion stroage and transport : ferritin, transferrin and cerculoplasmin. 5 hrs.

Meralloenzymes and coenzymes containing cobalt, iron and copper and their significance. Model compounds.

Nitrogen fixation : Nitrogen cycle, bacterial nitrogenase systems (*in vivo*), Synthetic studies (*in vitro*). 5 hrs.

Chlorophyll and its role in Photosynthesis

Oxygen carriers : Physiology of hemoglobin, and myoglobin, dioxygen binding, model compounds.

Electron transfer proteins : Cytochromes,ferrodoxins, rubredoxins

Non-porphyrin system : Hemerythrin and hemocyanin.

7 hrs.

*Books Recommended :*

1. Inorganic Chemistry, 4th Edn.J. E.Huheey, E. A. Keiter and R. S. Keiter. Addison-Wesley (1993).
2. Inorganic Chemistry, 2ndEdn. ( ELBS), D.F.Shriver, P.W.Atkins and C.H.Langford.
3. Concepts and models in Inorganic chemistry 3rdEdn. B.Douglas. D.H.Daniel and J.J.Alexander, John-Wiley and Sons (1983).
4. Concise Inorganic chemistry-J.D.Leee, 5th edn, New Age Interrnational (1996).
5. Inorganic chemistry-K.F.Purcell and J.C.Kotz (W.B.Saunders san Francisco).
6. Physical Inorganic chemistry, S.F.A. Kettle, Spektrum Academic Publishers Oxford.
7. Coordination Chemistry, D.Banerjea, New Age International
8. Symmetry and Spectroscopy of Molecules, K. VeeraReddy, New Age International(1998).
9. An Introduction to Bioinorgani Chemistry, R.J.P.Williams.
10. Inorganic Chemistry of Biological Processes, M.N. Hughes.
11. Principles of Bioniorganic Chemistry, S.J.Lippard and J.M.Berga. Panima Publishing Corporation.

## CHI-3.2 : Molecular spectroscopy and Diffraction methods.

Basic concepts and Introduction :

Properties of electromagnetic radiation ; Wave property-interference, diffraction.

Regions of the electromagnetic spectrum, energies corresponding to various kinds of radiation. Interaction of electromagnetic radiation with matter (absorption, emission, transmission, reflection, dispersion, polarization and scattering.)

General applications 3-hrs.

Electronic spectroscopy

A. Molecular electronic absorption spectroscopy. (UV-Visible)

Electronic spectra of diatomic molecules, electronic transitions, selection rules, assignement of transitions, band intensities, substituent and solvent effects, charge transfer transitions, Application to organic and inorganic molecules. 4-hrs.

B. Photoelectron spectroscopy.

Basic principles; Photo-electric effect. ionization process, Koopman`s theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.

Instrumentation.

Auger electron Spectroscopy-basic idea. 3-hrs.

Microwave spectroscopy : The rotation of molecules, rotational spectra, diatomic molecules, effect of isotopic substitution on transition frequencies, polyatomic molecules. Techniques and instrumentation. Stark effect, Applications; dipole moment, bond length.

3-hrs.

Vibrational spectroscopy

Infrared spectroscopy

Vibrational energy levels, infrared spectra of diatomic and polyatomic molecules, Normal modes of vibration, force constant, selection rules, anharmonicity, the vibration-rotation spectroscopy. Infrared spectra of simple molecules upon cordination compounds, changes in intrared spectra of donor molecules upon coordination in (N,N-dimethylacetamide, urea, Dmso, pyridine N-oxide, benzonitriles

etc), Change in spectra accompanying change in symmetry upon coordination($No_3^-$, $So_4^{2-}$, $N0^-_2$and $ClO_4^-$,) hydrogen bonding, instrumentation including FTIR
7-hrs.

Raman spectroscopy

Theory, relation with IR spectroscopy, resonance Raman, stimulated hyper and inverse Raman effects. Experimental techniques. Structure determination from IR and Raman spectra($CO_2$ ,$SO_2$, NO, $N_2O$, $OH_2$, $ClF_3$ and $NO_3$ ), use of lasers. 3-hrs.

Magnetic Resonance spectroscopy

A. Nucleat Magnetic Resonance(NMR) spectroscopy Magnetic properties of nuclei, population of energy levels, the Larmor precession, relaxation processes, chemical shift, sheilding mechanism, spin-spin interactions, rules governing the interpretation of first order spectra, effect of chemical exchange on spectra. Analysis of complex NMR spectra, $^1$Hnmr spectra of organic molecules and complex metal hydrides, NMR studies of nuclei other than proton, $^{13}$C, $^{19}$F, $^{31}$P, $^{11}$B and $^{15}$N, spectra of paramagnetic complexes, contact shift, double resonance technique, shift reagents, Instrumentation including FT nmr. 9-hrs.

B. Electron Paramagnetic Resonance (EPR) Spectroscopy

Basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of EPR spectra, hyperfine interaction, spin-orbit coupling, zerofield splitting and Karmer`s degeneracy, rules for interpreting spectra, factors affecting the magnitude of g values. Instrumentation. Applications to the study of free radicals, Coordination compounds, biological studies, rate of electron exchange reactions.
6-hrs.

C. Nuclear Quadrupole Resonance (NQR) Spectroscopy.

Quadrupole nuclei, Quadrupole moment, electric field gradients, The NQR experiment, structural information from NQR spectra. 2-hrs.

Mossbauer Spectroscopy

Indroduction, Principles, conditions for Mossbauer spectroscopy, parameters from Mossabauer spectra, isomer shifts, electric quadrupole interaction, magnetic interactions, Mossabauer spectrometer. Applications, $Fe_3(CO)_{12}$, Prussian blue, Oxyhemerythrin, Hexacyanoferrates, Nitroprusside, tin halides.
4-hrs.

X-Ray diffraction.

Origin and prodiction of X-Rays. Interaction of X-Rays with matter; absorption, scattering and diffraction., Crystal structure; The unit cell, Lattices, planes and Miller indices.

Reciprocal lattice- Bragg`s law in reciprocal space. Instrumentation : Sources, filters, monochromators and detectors.

Debye-Scherrer poweder methods, Weissenberg camera. General concept of solutions of Structure.

Applications : Analysis of structure, Crystal structures of NaCI and KCI. 6-hrs.

*Books Recommended*

1. Fundamentals of Molecular spectroscopy, C.N.Banwell
2. Physical methods in Chemistry, R.S.Drago, Saunder College
3. Structural methods in Inorganic Chemistry, E.A.Ebsworth, D.W.H. Rankin and S.Cradock, ELBS
4. Infrared spectra of Inorganic and coordination compond, Nakamoto.

5. Infrared spectroscopy, C.N.R.Rao.
6. Electron Absorption Spectroscopy and selected techniques. D.N.Satyanarayana, University Press India Ltd. Huderabad

CHOS 3.4 : Selected topics in Organic Chemistry. (See page 23)

CHPS 3.5 : Selected topics in Physical Chemistry. (See page 25)

CHI (Pr) 3.6 Lab course in Inorganic Chemistry

a). Preparation of selected Inorganic Compounds.

1. Copper-glycine complex : cis-and transforms.
2. N,N-bis(Salicylaldehyde)ethlinediamine cobalt complex. Oxygen takeup by Co(salen)
3. Co(DMG) model for Vit-B2 and reactions
4. CuCI2 -DMSO complex.
5. Tris(acetylacetonato) Cr(III)-Bromination reaction
6. Phenyl mercuri acetate
7. Chloropentammine cobalt (III) chloride.
8. Nitro-and nitrito complexes.
9. Separation of optical isomers of cis [Co(en)2 CI2]CI.

(b) Characterization

1. Elemental Analysis of above complexes : $N_2$ by Kjeldhal`s method, metal and anion estimation. IR, Electronic, NMR, Magnetic studies of above complexes.
2. Interpretation of IR and NMR spectra.
3. Homeogeneous catalysis by $CoBr_2$ conversion of p-xylene to terphthalic acid.
4. Measurement of band gap of a semiconductor.
5. Meisener Effect (demonstration)
6. Reaction of Cr(III) with murtidentate ligand. A kinetics experiment visible spectrum of Cr(EDTA) complex.

Scheme of Examination Duration 7 hours

| | | |
|---|---|---|
| 1. | Preparation of a complex | 30 |
| 2. | Analysis or determination from a pure complex | 20 |
| 3. | Interpretation of a given spectrum | 20 |
| 4. | Viva | 05 |
| 5. | Records | 05 |

CHI- (Pr) 3.7 Lab Course in Inorganic Chemistry

Instrumental methods of analysis

a). Colorimetry

1. Determination of Fe by o-Paenhnthroline
2. Determination of Zr by Alizarin red S
3. Determination of Ti by $H_2$ $O_2$method
4. Determination of Mn/Cr/V in steel samples
5. Determination of composition of Fe-ophen complex by Job`s method
6. Mole ratio method Zr + Alizarin red-S
7. Slope ratio method Cu + en complex
8. Determination of stability constant of (7).
9. Determination of pKa of an indicator (methyl red) in aqueous solution

b) Conductometry

c) Potentiometry

d) Electrogravimetric analysis

e) Magnetic susceptibility determination.

f) Flame photometry

| Scheme of Examination | Duriation 7 hours |
|---|---|
| 1. Colorimetry | 40 |
| 2. | One of b/c/d/e/f 30 |
| 3. | Viva 05 |
| 4. Records | 05 |

*Books Recommended*

1. Vogel`s Text Book of Quantitative Inorganic Analysis, J. Bassett, R. C. Denney, G.H. Jaffery and J. Mandham, Longmans, Green and Company Ltd.

2. Preparative Inorganic Chemistry, Brauer

3. Practical Inorganic Chemistry, G.Pass and H.Sutcliff, Chapman and Hall Ltd. (1968)

4. Standard Methods of Chemical Analysis- W.W.Scott and N.H. Furnan.

## ORGANIC CHEMISTRY

CHO-3.1 : Stereochemistry, reaction mechanism and Spectroscopy.

1. Dynamic stereochemistry- I : Stereoselective reactions. Principle of Stereoselectivity.

Asymmetric synthesis and asymmetric induction. Acyclic stereo selection, diastereo selection in cyclic systems Enantioselective synthesis.

10 hrs.

2. Reaction Mechanism-I. Methods of determining reaction mechanisms. Product studies, cross-over experiments, isotopic labelling, stereochemical and kinetic studies. *Kinetically and thermodyamically Controlled products.* Intermediates VS transition states.

$S_N1$ and $S_N2$ reactions. Substitution at allylic carbon. Neighbouring group participation.

Reactive intermidiates: Formation, Structure, Stability and reactions of carbenes, nitrenes and enamines. 10 hrs.

3. Spectroscopic Methods. Expression of electromagnetic radiation in terms of wavelength, wave number and frequency. Relation of these parameters with energy.

Ultraviolet and visible spectroscopy : Theory of electronic excitation. Application of Beer-Lamberts law. Instrumentation. Chromophores and auxochromes. Spectral

correlations of conjugated compounds, enones and related compounds, and aromatic compounds. Wood ward-Fieser rules for calculation of max. Effect of solvents and steric effects. Problems. Optical Rotatory dispersion : Theory of optical rotation. Octant rule, Cotton effect and haloketone rule. Relation between Cotton effect curves and structure. Application of ORD to structural problems.

Infrared spectorscopy : Molecular vibrations. Concept of group frequencies.

Factors affecting the group frequencies : bond order, mass effect (Hookes law), inductive, resonance, steric effects and intramolecular interactions. Fermi resonance. Instrumentation. Discussion of IR bands associated with common functional groups. Study of hydrogen bonding Problems.

10 hrs.

Nuclear Magnetic Resonance Spectroscopy : Theory of nuclearresonance. Chemical shift and factors affecting chemical shifts. Instrumentation. Diamagnetic and paramagnetic anisotropies. First order and second order spin-spin coupling. Types of spin-spin coupling and factors affecting the coupling constants. Fourier Transformation. Techniques for simplification of spectra (Double resonance, NOE, INDOR CIDNP) Interpretation of spectra. Applications and problems.

Dynamic NMR : Exchange Phenomenon, Temperature effects.

Carbon-13 NMR-Introduction, Comparison with 1H-NMR spectroscopy. Interpretation of the data, applications & problems. COSY & NOSEY NMR spectra.

10hrs.

Mass spectrometry : Principles of mass spectrometry. Instrumentation. Different methods of ionisation. Determination of molecular formula by accurate molecuar weight and isotope abundance methods. Fragmentation, Nitrogen rule, Metastable ions. Fragmentation of a) normal and branched alkanes.(b) alkenes (c) benzene and its derivatives (d) alcohols (e)aldehydes & Ketones (f) acids and esters (g) ethers (h) amines (i) halides (j) nitrocompounds. Mass spectral fragmentation of Pyrrole, Furan, Thiazole, Pyridine, Indole, Coumartin. Composite problems involving UV,IR, NMR, and Mass techniques.

10 hrs.

*Books Recommedended*


1. Sterecohemistry by E.Eliel. Tata Mc Graw Hill, New Delhi (1992)
2. Stereochemistry- Conformation and Mechanism by P.S.Kalsi, Wiley-Eastern Ltd, New Delhi (1992).
3. Stereochemistry by D.Nasipuri,. New Age International 2nd Edition New Delhi (2000).
4. Organic Chemistry- Vol. I & II by I.L.Finar 6th Edition. 1998. ELBS London.
5. Advanced Organic Chemistry by F.A.Carey, Mc Graw Hill, 4th Edition, New York (1987)
6. Organic Chemistry by T.N. Sorrel, Uni.Sci.Books California USA (1999).
7. Advanced Organic Chemistry (reaction Mechanism) By Jerry March 3rd Edition, Wiley Estern Ltd
8. Theory and Mechanism in Organic Chemistry by Lowery and Richardson.
9. Organic Chemistry Vol.I & II & III.Mukherjee, Kapoor & Singh. Wiley Estern Ltd.(1992)
10. Absorption Spectroscopy of Organic Molecules by V.M. Parikh, Addison Wesely.
11. Spectroscopic Identification of Organic Compounds by Bassler, Silverstein and Morrill.
12. Spectroscopic Methods in Organic Chemistry, by Dudley H. Willams and Ian Fleming Tata Mc Graw Hill (1988)

13. Organic Spectroscopy by D. W. Brown, A. J. Floyd and M. Sainsbury John Wiley and Sons.
14. Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry by L.M. Jackmann and Sternhell. Pergamon Press, London (1969).
15. Carbon-13 Nuclear Magnetic Resonance Spectroscopy, by G.C. Levy, R.L. Linchter and G.L.Nelson, Johns Wiley &Sons, N.Y. (1980).
16. Interpretation of Mass Spectra by McLafferty.
17. Organic Mass Spectroscopy by Das and James.
18. Mass Spectra of Organic Compounds, by H. Budzikiewicz, C.Djerassi and D.H. Williams Holden- Day, Sanfrancisc (1967).
19. Optical Rotatory Dispersion by C. Djerassi, McGraw-Hill Book Company, New York (1960).
20. ORD and CD in Chemistry and Biochemistry by O.Crabbe, Academic Press Inc, New York (1972).
21. Spectroscopy of Organic Compounds By P.S.Kalsi, New Age international 4th Edition, New Delhi (1999)

CHO 3.2 : Aromaticity and natural products.

1. Aromaticity : HMO theory of aromaticity, REPE Application of physical methods (UV,IR,PMR and X-ray) in the study of aromaticity of: cyclopropyl, cyclopentyl, cycloheptatrienyl ions. Cyclooctateraenyl dianion, [10].[12], [14], [16], and [18] annulenes. Heteroannulenes. Antiaromaticity and homoaromaticity with examples.
   10 hrs.
2. Steriods : Sterols and bile acids : Structure, Synthesis and biological properties of Cholesterol, Cholic acid and Ergesterol. Conformation of steroidal skeleton. Photochemical reactions of Vitamin D-group. Biogenesis of Cholesterol.
   10 hrs.
3. Steroidal hormones : Estrogenic hormones-Estrone, Estradiol. Estriol Androgenic hormones- Androsterone, testosterone. Corpus Luteum hormones- Progestrone.
   Adrenal cortex hormones- Cortison and aldosterone. (Barton`s photochemical systhesis) Transformation of Cholesterol, and Ergosterol to Progesterone.
4. Terpenes : General Introduction.

Bicyclic sesquiterpenoids : Cadinene, Edesmol, Caryophylline, Tricyclic sesquiterpenoids : Cedrene. Triterpenoids : Squalene.

Biosynthesis of terpenoids : Citronellal, terpeneol and pinene. 10 hrs.

5. Heteroyclic- compounds I

Structure, reactivity, ring synthesis, reactions and medicinal uses of the following heterocycles :

Three and four membered- heterocycles with one heteroatom-Oxiranes, aziridines, thiiranes, oxetanes, azetidines and thietanes.

10 hrs.

*Books Recommended*

1. Aromaticity by R.J.Garrat.
2. The aromatic sextet, G.E.Clark.
3. Organic Chemistry by F. A. Carey & Sandburg.
4 Organic Chemistry by I.L.Finar, Vol II 6th Edition ELBS London 1998
5. The Alkaloids, Vol II-IV by K.W. Bentley.

6. The Chemistry of Alkaloids by S.W. Pelletier.
7. Terpenoids Vol-I, II by P. De Mayo.
8. Heterocycles. An Introduction of the Chemistry of Heterocyclic Compounds, by R.M.Acheson. John Wiley and Sons 4th Edition.
9. Heterocyclic Chemistry by A.R. Katritzky & J.J. Logowskii Methuen.
10. Heterocyclic Chemistry by T. Gilchrist, Butterworths London (1985).
11. Modern Heterocyclic Chemistry by Joullie and Smith.
12. Heterocyclic Chemistry by R. K. Bansal. Tata Mc Graw Hill, New Delhi (1999).

CHIS 3.3 Selected topics in inorganic chemistry. (See page 38)

CHPS 3.5 : Selected topics in physical chemistry. (See page 41)

Practicals

CHO (Pr)-3.6 Practical-I

Qualitative analysis of Ternary mixture.

CHO(Pr)-3.7 Practical-II

Preparation of three Derivatives.

Estimation of Glucose

Scheme of Examination

| CHO(Pr)-3.6 Practical-I | Duration 7 hrs |
|---|---|
| Qualitative analysis of Ternary mixture | 70 marks |
| Journal | 05 marks |
| Viva | 05 marks |
| Total | 80 marks |

| CHO (Pr)-3.7 Practical-II | Duration 7 hrs |
|---|---|
| Preparation of three Derivatives | 55 marks |
| Purification and physical constants | 15 marks |
| Journal | 05 marks |
| Viva | 05 marks |
| Total | 80 marks |

## PHYSICAL CHEMISTRY

CHP 3.1 : Quantum Mechanics, Atomic Structure and Atomic Spectra Quantum Mechanics

Review of Classical mechanics : Equation of motion for a particle Newtonian, Lagrangiana and Hamiltonian equations of motion, elementary wave motion. 4 hrs.

Postulates of quantum mechanics, operators, eigen values and expectation values. Commuting operators and Hermitian operators, time dependence of wave functions.

Application of Schrodinger equation : Review of the results of particle in a box of one -, two-and three dimensions, degeneracy. Reflection and penetration of a particle in a one dimensional box of semiinfinite barrier, a particle in a box of finite walls, linear harmonic oscillator Hermite Polynomials. A rigid planar rotator,derivation of selection rules for transitions in rotating molecule. The rigid rotator with free axis and the orbital angular momentum operators.

Equation for hydrogen atom and its solutions, separation of variables, the phi, theta and radial equations, the problems of spherical symmetry. Electronic quantum numbers and electron spin 20 hrs.

Approximate methods in quantum mechanics :

(1) Variation method and its application to hydrogen atom, secular equations and secular determinants, application of variation method to hydrogen molecule ion, hydrogen molecule and normal helium atom.

(2) Perturbation theroy and its application to linear harmonic oscillator.

8 hrs.

Atomic Structure and Atomic Spectra

A summary of the hydrogen spectrum. Alkali spectra and alkali like spectra, spark spectra and arc spectra. Moseley lines.

Helium and alkaline earth spectra. Multiplet structure of line spectra. Doublet structure of alkali spectra and compound doublets, triplets and singlets of alkaline earths and helium, prohibition of intercombinations. Multiplicities and term symbols.

Space quantization : Zeeman effect, normal and anomalous Zeeman effects, Paschen- Back effect, Stark effect. 18hrs

50hrs

*Books Recommended*


1. Quantum Mechaincs -L.T.Schiff, Prentice-Hall.
2. Quantum Chemistry- H. Eyring, J.Walter and G.E.Kimball, John Wiley.
3. Quantum Mechanics-An introduction- H.L.Strauss, Prentice Hall of India.
4. Quantum Mechanics-L.Pauling and E.B.Wilson, McGraw hill.
5. Contemporary Quantum Chemistry-J.Goodisman, Plenum/Rosetta.
6. Quantum Chemistry- K.S.Pitzer, Prentice-Hall
7. Introductory Quantum Mechanics-Valdimir Rojanstry.
8. Quantum Chemistry- John P.Lowe.
9. Physical Chemistry- P.W. Atkins, Clarendon Press, Oxford, 1970.
10. Molecular Quantum Mechanics-P.W.Atkins, Clarendon Press, Oxford, 1970.
11. Introduction to Quantum Chemistry-J.M.Anderson.
12. Introduction to Quantum Mechanics-R.H.Dicke, J.P. Wittke.
13. Indroductory Quantum Chemistry- A.K,Chandra, Tata Mc Graw Hill New Delhi 1994.
14. Quantum Mechanics in Chemistry-M.W.Hanna.
15. Quantum Chemistry, R.K. Prasad, New Age International Publishers, New Delhi.
16. Atomic Spectra and Atomic structure, G.Herzberg, Van Nostrand


CHP-3.2 : Molecular Structure-I

1. Rotation of Molecules and Rotational Spectra

Classification of molecules; momental ellipsoid, energy levels of linear, symmetric, spherical, and asymmetric top molecules and their symmetry properties. Thermal distribution of rotational energy levels. Infrared rotational spectra, non-rigid rotor treatment. 8 hrs.

2. Vibrations of Molecules

Molecule as harmonic oscillator : vibrational eigen functions and eigen values. Hermite polynomials; calculation of transition of probabilities and selection rules. The anharmonic oscillator, energy levels, selection rules and I.R.Spectra. Mathematical form of potential energy curves. Rotation - vibration spectra, shapes of absorption bands in case of (i) linear, (ii)symmetric top, (iii) sphjerical top and (iv)asymmertic top, molecules. Isotopic effects. Applications of I.R. spectroscopy

8 hrs.

3. Microwave Spectroscopy

Gaseous microwave spectra and rotational transitions : Study of inversion of ammonia and hindered rotations in molecules. Instrumentation. Stark effect in molecular spectra; first and second order Stark efects. 6 hrs.

4. Nuclear Magnetic Resonance

Magnetic properties of nuclei, theoretical principles underlying NMR and experimental set up. Shielding and deshielding mechanisms and concept of chemical shift. High resolution NMR. Spin-spin coupling, coupling constants and elucidation of structure by NMRspectra. Kinetic applications. 15 hrs.

5. Nuclear Quadrupole Resonance Spectroscopy

Theory and instrumentation. Effect of magnetic field on the spectra, relationship between electric field gradients, q and molecular structure. Applications. The interpretation of eQq. data effec t of crystal latties on the magnitude of EQq Structural information from NQR spectra. 5 hrs.

6. Optical Rotatory Dispersion and Circular Dichroism

Simple theoretical account and instrumentation. Treatment of data, applications to gross structure determination, octant rule, determinationof stereochemistry and absolute configuration. 8hrs

Total : 50 hrs

*Books Recommended*


1. Introduction to Molecular Spectroscopy, G.M.Barrow, McGraw Hill
2. Physcial Methods in Inorganic Chemistry, R. S. Drago East-West Press, New Delhi.
3. Molecular Spectroscopy, J D. Graybeal. McGraw Hill
4. Spectroscopy, Volume I,II,III Ed B.P. Straughan and S. Walker Chapman Gall, 1976.
5. Molecular Magnetic Resonance Spectroscopy, R.M.L.Bell and R.K. Harris
6. Spectra of Diatomic Molecules, G. Hertzberg, D. Van Norstrand Co. Inc. Prenceton N.J. 1950
7. Infrared and Raman Spectra of Polyatomic molecules, G.Hertzberg, D. Van Norstrand Co.Inc. Prenceton N.J. 1950
8. Absorption Spectroscopy, R.P.Bauman.
9. Molecular' Structure : A Physical Approach, J.C.D. Brand and J.C. Speakaman, Edward Arnold Ltd., London.
10. Microwave Spectroscopy, J.M. Sugden and C.N. Kenny.
11. Fundementals of Molecular Spectroscopy, C,N.Banwell, Tata- Mcgraw Hill, New Delhi, 1975.
12. Microwave Spectroscopy, D. Gordy, W.V.Smith and R.F.Trambarulo, John Wiley and Sons, N.Y. 1969.
13. Molecular Vibrations, E.B.Wilson, J.C. Decius and P.G.Cross.
14. Nuclear Magnetic Resonance, E.R.Andrew, Chambridge University Press, Cambridge, 1955.
15. Nulcear Magentic Resonance, J.D. Roberts, McGraw Hill Book Co. N.Y. 1959.
16. Microwave Spectroscopy, C.H. Townes and A.L. Schawlow, McGraw Hill Book Co. N.Y. 1955.
17. Treatise on Physical Chemistry, H.S.Taylor and S. Glasstone, Vol. I and II, D.Van Nostrand, N.Y. 1957.

18. Basic Principles of Spectroscopy, Raymand Chang. McGraw Hill, Kogakusha Tokyo, 1971.
19. Theoretical Chemistry, S. Glasstone.
20. Instrumental Methods of Analysis, Willard, Merit and Dean, Tata McGraw Hill, New Delhi, 1993.
21. Introduction to Magnetic resonance, A Carrington and A.D.. Mclachlan, Harper Rao.

CHIS 3.3 : Selected topics in Inorganic Chemistry. (See page 38)

CHOS 3.4 : Selected topics in Organic Chemistry. (See page 40)

CHP(Pr)-3.5 : Lab. Course in Physical Chemistry

1) Viscosity :

Molecular weight of a high polymer by viscosity determination.

2) Surface Tension

a) Variation of surface tension of aqueous solutions of a liquid (npropyl alcohol) with concentration and determination of limiting cross sectional area of the alcohol molecule.

b) Interfacial tension between two immiscible liquids(e.g benzene & water at room temperature)

3) Solubility

Heat of solution (e.g.oxalic acid, benzoic acid etc.) by solubility experiments.

4) Phase Equilibria

a) Distribution of benzoic acid (or succinic acid) between benzene and water.

b) Molecular weight of benzene (or nitrobenzene) by steam distillation.

c) Vapour pressure of chlorobenzene by steam distillation.

5) Thermochemistry

a) Heat of neturalization of strong acid.

b) Heat of neutralization of weak acid.

6) Refractometry

Electron polarization and electron polarisibility of a liquid.

7) Polarimetry

Precentage composition of two optically active substances (e.g,d- sucrose and d- trataric acid)

8) Absorptiometry

a) Applicability range(for an absorbing substance in solution and evaluation of absorbancy index, measuring unknown concentration.

b) Mixture analysis by absorptiometry.

c) Application of Hemmett Acidity function.

9) Electrolytic Conductance

a) Verification of the Onsagr equation as applied to electrolytes.

b) Comparision of strengths of weak acids (e.g.chloroacetic acid and acetic acid).

c) Conductometric titrations :

i) Weak acid Vs weak base, ii) $H_2SO_4$ Vs $BaC1_2$

iii) Moderatley weak acid like salycylic acid Vs NaoH (Salt line method and alkali method),

iv) Dilute solution of a weak acid (0.01 to 0.001N)Vs NaoH by addition of solvent of low dielectric constant, using ammonia and NaOH titrants and by double alkali method.

10) Transference member of H+ and CI ions by moving boundary method.

11) Reaction Kinetics

Hydrolysis of methyl acetate : i) catalytic coefficients (or strengths of acids)

ii) Arrhenius parameter iii) Degree of Hydrolysis of Urea hydrochloride using HCl & equinormal urea hydrochloride solutions.

12) Emf of cells

a) Standard electrode potential of reversible metal- metal ions at room temperature.

b) Solubility of sparingly soluble salts

c) Dissociation constants of a weak monobasic acid

d) Acid and base dissociation constants of an amino acid and its iso-electric point.

e) Titration of $Fe^{2+}$ with $Ce^{4+}$ and determination of the formal redox potential of $Fe^{3+}/Fe^{2+}$ and $Ce^{4+}/Ce^{3+}$.

13) Cryoscopy

Determination of cryoscopic constant of the given solvent.

*Books Recommended*


1. Findlay`s Practical Physical Chemistry, 9th edition, revised by B.P.Levitt.
2. Practical Physical Chemistry by A.M.James and F.E.Prichard
3. Experiments in Physical Chemistry by Shoemaker and Garland
4. Experiments in Physical Chemistry by Daniels, Alberty and Williams et.al.
5. Laboratory Physical Chemistry by Oelke/ M.A.C.T.L.A.C.
6. Experimental Physical Chemistry by W.G. Palamer
7. Advanced Physico-chemical experiments by J.Rose
8. Experimental Physical Chemistry by V.D.Athwale and Paul Mathur, New Age International Publishers.
9. Text book of Physical Chemistry by S.Glasstone
10. Text book of quantitative analysis by A.I.Vogel
11. Advanced Practical Physical Chemistry by J.B. Yadhav, Goel Publishing house, Meerut.


Scheme of Examination (Short Exercise)

CHP(Pr)-3.5

Duration of Examination _____7 hours

a) Experiment I _____35 marks
b) Experiment II _____35 marks
c) Viva_____05 marks
d) Journal_____05 marks

## CHP(Pr)-3.6 : Lab. Course in Physical Chemistry

1) Viscosity :

Viscosity of air by Rankine`s method

2) Surface Tension :

a) Effect of added salt on the surface tension of water
b) Critical micelle concentration of a soap molecule. (e.g. Potassium laureate).

3) Solubility :

Effect of addition of an electrolyte on the solubility of an organic acid.

4) Phase Equilibria :

Equilibrium constant of the reaction : KI +I2 $KI_3$ and the determination of an unknown concentration of KI solution.

5) Thermochemistry :

a) Heat of hydration of $CuSO_4$(heat of crystallization of $CuSO_4.5H_2O$)
b) Integral heat of solution and dilution of salts (e.g.$KNO_3$,NaCI etc.)

6) Refractometry :

Variation of refractive index with composition of mixture (e.g.$CCI_4$ and $CH_3COOC_2H_5$)

7) Absorptiometry :

a) Absorptiometric titration of hydrochloric acid
b) Absorptiometric estimation of Fe (III) with EDTA.

8) Electrolytic Conductance :

Equivalent conductance of a weak acid, e.g. acetic acid at different concentrations and testing the applicability of Ostwald`s dilution law.

9) Mobilities of ions

a) Transference numbers of silver and nitrate ions in a solution of silver nitrate by Hittorff 's method.

10) Reaction Kinetics

a) Reaction kinetics of $H_2O_2$ and HI: Clock reaction b) Salt effect on the persulaphate oxidation of iodide ion.
c) Auto catalysis : Mn(VII) oxidation of oxalic acid in the presence of $H_2SO_4$
d) Kinetics of decomposition of the complex formed between sodium sulphide and sodiumnitroprusside

11) Emf of cells

a) Mean ionic activity coefficent of hydrochloric acid at different concentrations using a concentration cell without transference: influence of ionic strength on the mean ionic activity coefficient.
b) Degree of hydrolysos and $K_h$ of aniline hydrochloride.
c) Stability constants of Cu 2+ - EDA complex.
d) Ionic product of water at 25OC
e) Titration of $H_3PO_4$ with NaOH
f) Titration of Zn(II) with K4Fe(CN)$_6$ and verification the formula of the complex formed between Zn(II) and $Fe(CN)_6^{4-}$.

12) Cryoscopy :

Determination of activities of an electrolyte and a nonelectroylte by cryoscopic method.

*Books Recommended*

1) Findlay`s Practical Physical Chemistry, 9th edition, revised by B.P. Levitt.
2) Practical Physical Chemistry by A.M. James and F.E.Prichard

3) Expremients in Physical Chemistry by Shoemaker and Garland
4) Experiments in Physical Chemistry by Daniels, Alberty and Williams et.al.
5) Laboratory Physical Chemistry by Oelke/M.A.C.T.L.A.C.
6) Experiments in Physical Chemistry By W.G.Palmer
7) Advanced Physico-Chemical Experiments by J.Rose
8) Experimental Physical Chemistry by V.D. Athwale and Paul Mathur, New Age International Publishers.
9) Text book of Physical Chemistry by S. Glasstone
10) Text book of quantitative analysis by A.I.Vogel
11) Advanced Practical Physical Chemistry by J.B.Yadhav, Goel Publishing house, Meerut

Scheme of Examination (Long Exercise)

CHP(Pr)-3.6

Duration of examination_____ 7hours

a) Experiment_____70 marks
b) Viva_____ 05 marks
c) Journal_____05 marks

CHIS-3.3 : Selected topics in Inorganic Chemistry

1. Instrumental methods of analysis

(a). Thermogravimetry, Thermobalance, factors influencing results of thermogravimetry. Differential thermal analysis, instrumentation for differential thermal analysis and DSC. Application of TG.DTA & DSC,
4 hrs.

(b). Flamephotometry, Principles, flame photometers, interference, standard addition method and internal standard method. Applications.
2 hrs.

(c). Atomic Absorption spectrometry, Principles, advantages over flame emission spectrometry, instrumentation for AAS, non flame techniques for atomization, Vapour generation technique and applications.
2 hrs.

(d). Separation techniques and applications:

(i). Gel filtration
(ii). Electrophoresis
(iii). Stripping Voltammetry.
(iv). Cyclic Voltammetry. 4 hrs.

2. Advanced coordination chemistry : Review of theories, ligandfield theory, evidences for metal-ligand orbitals overlap, Spectroscopic ground state terms, Selection rules Interpretation of electronic spectra

($d^1$-$d^6$ systems) using Orgel and Tanabe-Sugano diagrams, Racah parameters, charge- transfer spectra.

Types of magnetic behaviour, TIP,orbital contribution, quenching of orbital moment, diamagnetic corrections, Spin cross over in complexes, magnetic susceptibility determination by Gouy method. 10 hrs.

3. Reactions mechanism of coordination compounds : Fundamentals of mechanistic concepts : Electron transfer reactions, mechanism of electron transfer recation; Outer sphere and inner sphere electron transfer. Complimentary and non-complimentray reactions. Synthesis using electron transfer reactions.
5 hrs.

Substitution reactions : Classification of ligand substitution mechanism, Substitution reactions in octahedral complexes : Acid hydrolysis, base hydrolysis, anation reactions, Substitution reactions in square planar complexes : cis and trans effect. Synthesis of coordination compounds by substitution reactions.(brief survey) 4 hrs.

4. Bioinorganic chemistry : Metal ions in biological systems, cell, significance of ionosphores, ion transport across membrances ($Na^+$,$K^+$). Chlorophyll and its role in photosynthesis. Nitrogen fixation (in vitro and in vivo). Oxygen uptake proteins-haemoglobin and myoglobin. Electron transfer proteins- cytochromes, rubredoxins, ferrodoxins and Vit$B_{12}$ 10 hrs.

5. Organometallic chemistry of transition elements : Synthesis, structure & bonding, . Organometallic in Organic synthesis and homogeneous catalysis reactions (hydrogenation, hydroformylation, isomerisation and polymerization); Pi-acid metal complexes. Activation of small molecules by coordination. 6 hrs.

6. Superconductors : Type I and Type II, Superconductors metal oxides, organic compounds. Applications. 3 hrs.

*Books Recommended*


1. Thermal Methods of Analysis, W.W.Wendlandt
2. Instrumental Methods of Analysis , H.W.Willard, L.L.Merrit, J.A. Dean and F.A.Settle
3. Introduction to Instrumental Analysis, R.D.Braun.
4. Chromatography, Erich Heptaman
5. Instrumental Methods of Analysis, B.K.Sharma
6. Inorganic Chemistry, 4thEdn. J.E.Huheey, E.A.Keiter and R.S. Keiter. Addission-Wesley (1993).
7. InorganicChemistry, 2nd Edn. (ELBS), D.F. Shriver, P.W.Atkins and C.H. Langford. Oxford University Press (1994)
8. Concepts and models in Inorganic Chemistry 3rd Edn. B.Douyglas.,D.H.Daniel and J.J. Alexander,John-Wiley and Sons (1983).
9. Concise Inorganic Chemistry- J.D.Lee, 5th Edn, New Age International (1996).
10. Inorganic Chemistry- K.F.Purcell and J.C.Kotz (W.B.Saunders san Francisco).
11. Physical Inorganic Chemistry, S.F.A.Kettle,Spektrum Academic Publishers Oxford.
12. Coordination Chemistry, D.Banerjea, New Age International.
13. Symmetry and Spectroscopy of Molecules, K.VeeraReddy, New Age International (1998).


CHOS 3.4 : Selected topics in organic chemistry

1. Stereochemistry : Stereoselective reactions : Principles and terminology. Addition of nucleophiles to carbonyl compounds, catalytic hydrogenation, Epoxidation. 10 hrs.

2. Reaction mechanism : Use of kinetic and non-kinetic methods in determination of organic reaction mechanism. Kinetic isotope effects. A study of the following named reactions : Darzen`s reaction, Favorskii rearrangement, Baeyer-Villiger reaction, Fries, Houben-Hoesch reaction, Claisen ester condensation, Claiser-Schmidt reaction,-Beckmann and Favorskii rearrangement. 10 hrs.

3. Elementary aspects of Pericyclic reactions and Photochemistry.

Introduction and Classification : Electrolytic reactions Woodward-Hoffmann rules

Principles of Photochemistry : Photochemistry of carbonyl group-Norrish Type-I, and Type-II cleavages. Paterno-Buchi reaction. 10 hrs.

4. Retrosynthetic Analysis and Reagents.

Strategy of organic Synthesis : Introduction, terminology and application to simple aromatic compounds.

Synthetic uses of : Organoborane, Organo magnesium and Organolithium compounds in Organic sysnthesis 10 hrs.

5. Application of spectroscopic methods to structure elucidation of simple organic molecules.

Use of IR, NMR and Mass spectroscopic methods for characterisation of simple organic molecules. Composite problems.

10 hrs.

*Books Recommended*


1. Stereochemistry by E.Eliel, Tata McGraw Hill, New Delhi, (1992)
2. Stereochemistry by D.Nasipuri.2nd Edition New Age International New Dehi, (1999)
3. Advanced Organic Chemistry by Jerry March, 3rd Edition Wiley Estern New Delhi (1984)
4. Organic Synthesis- The Disconnection Approach by S. Warren. Designing Organic Synthesis by Stuart Warren.
5. Modern Synthetic Organic Chemistry by H.O.House W.A.Behjamin INC, New York (1969)
6. Molecular Photochemistry byy N.J.Turro.
7. Molecular reactions and Photochemistry by Depoy and Chapman
8. Organic Photochemistry by J.M.Coxan and B.Halton Cambridge University press London, (1974)
9. Spectroscopic Identification of Organic Compounds by Bassler, Silverstein and Morrill.
10. Spectroscopic Methods in Organic Chemistry, by Doudley H. Willams And Ian Fleming Tata McGraw Hill (1988)
11. Organic Spectroscopy by D.W.Brown,A.J. Floyd and M.Sainsbury John Wiley and Sons.
12. Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry by L.M.Jackmann and Sternhell. Pergamon Press, London (1969).


CHPS 3.5 : Selected Topics in Physical Chemistry

1. Physical Properties of Molecules

Optical avtivity, polarization-(Clausius Mossotti equation), orientation of dipoles in elecrtic field, dipole moment, induced dipole moments, measurement of dipole moments.

Magnetic properties-paramagnetism, diamagnetism and ferromagnetism. 6 hrs.

2. Introduction to Exact Quantum Mechanical results.

Approximate methods : The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Application of variation method and perturbation theory to helium atom. 05 hrs

3. Molecular Orbital Theory :

Huckel molecular/orbital theory of conjugated systems, bond order and charge density calculations. Application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene, etc. Introduction to extended Huckel theory.

05 hrs

4. Statistical Thermodynamics :

Concept of distribution : Ensemble averaging. Postulates of ensemblage averaging, grand canonical and micro canoncial ensembles, corresponding distribution laws (using Lagrange`s method of undetermined multipliers).

Partition Functions : Translational, rotational, vibrational partition functions.

Calculation of thermodynamic properties in terms of partition functions.

Applications of partition functions.

Heat capacity behaviour of solids. Chemical equilibria and equilibrium constants in terms of partition functions. Fermi-dirac statistics, distribution law and application to an alkali metal. Bose-Einstein statistics-distribution law and application to helium

14 hrs

5. Electrochemistry :

Electrochemistry of solutions : Debye Huckel-Onsagar treatment and its extension, ion-solvent interactions, Debye-Huckel-Bjerrum Model.

Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess). Methods of determining the structure of electrified interfaces. Guoy-Chapman, Stern, Graham- Devanathan-Mottwatts, Tobin, Bokris, Devanathan models.

Over potentials,exchange current density. Derviation of Butler-Volmer equation. Tafel plot.

Quantum aspects of charge-transfer at electrode-solution interface, quantisation, charge-transfer, tunneling. 10 hrs

6. Reaction Dynamics :

Absolute reaction rate theory. Effect of solvent, pressure and ionic strength for ion-ion, ion-neutral molecule type reactions, cage effect.

Homogemeous catalysis, kinetics of enzyme reactions, generalfeatures of fast reactions, study of fast reactions by flow method, relaxation method, Flash photolysis and the nuclear magnetic resonance method. 10 hrs

Total 50 hrs

*Books Recommended*


1. Physical Chemistry, G.M.Barrow, McGraw Hill
2. Physical Chemistry, R.A. Alberty, Wiley Eastern Ltd.
3. Elements of Physical Chemistry, P.W.Atkins, Oxford
4. Physical Chemistry by P.W. Atkins, ELBS.
5. Introduction to Quantum Chemistry, A.K.Chandra, Tata McGraw Hill
6. Quantum Chemistry, Ira N.Levine, Prentice Hall.
7. Modern Electrochemistry Vol.I and II, J.O.M,Bokris and A.K.N.Reddy,Plenum.
8. An Introduction to Electrochemistry, S.Glasstone, Van Norstrand, 1942.
9. A Text Book of Electrochemistry, G.F.A.Kortum and J.O.M. Bokris, Elsevier, 1951.
10. Electrolyte Solutions, R.A.Robinson and R.H.Stokes, Acedemic Press, 1959.

11. Chemical Kinetics, K.J.Laidler, McGraw Hill, 1950.
12. Kinetics and mechanism of chemical transformations, J.Rajaraman and J. Kuriacose, McMillan.
13. Theory of rate processes, S. Glasstone, K.J.Laidler and H.Eyring, McGraw-Hill,1941.
14. Thoeries of Chemical recation Rates, K.J.Laidler, Mc_Graw-Hill, 1969.
15 Fast Reactionss, D.N. Hague, Wiley-Interscience, New York, 1971.
16. Techniques of Oraganic by Weissberger(ed.), Interscience, 1963, Vol.VIII
17. Kinetics of Chemical Changes in Solution, E.S.Amis, McMillan, 1948
18. The Foundations of Chemical Kinetics, S.W. Benson, McGraw-Hill, 1960.

## SEMISTER- IV

## INORGANIC CHEMISTRY

CHI-4.1 : Instrumental Methods of Analysis.

1. Polarography : Theory, Instrumentation, diffusion and limiting current, half wave potential, DME, oxygen interference, methods of measurement of diffusion current, shape of polarographic maximum. Derivative polarography, anode waves, and anodic-cathodic waves.

4 hrs

2. Amperometric Titrations : Principle, Methodology, apparatus, pm, Successive titrations, titration to zero current, comparison with other titration methods. 2 hrs

3. Coulometry : Fundamental principles, apparatus, coulometers, constant current and controlled potential coulometry stripplng analysis and applications. 3 hrs

4. Ion Selective Electrodes : Terminology, Types and construction of ion selective electrodes ; glass electrode, solid state and precipitate electrodes, enzyme and gas sensing electrodes, glass microelectrodes and applications. 4 hrs

5. Conductometry : Introduction, important laws, definitions and relations,effect of dilution, conductance measurements and applications 2 hrs.

Separation methods

1. Gel filtration : Introduction, type of gels,techinques, use in equilibrium studies, estimating size, parameters, molecular weight determination, separating plant extract. 2 hrs

2. Electrophoresis : Introduction, varieties, techniques and applications. 2 hrs

3. Anodic/Cathodic stripping voltammetry 2 hrs

4. Cyclic voltammetry : 2 hrs

5. Flow injection analysis : Principles, chemical separation, development of flow injection analysis procedure, advantages, limitations and applications, 3 hrs

Spectral methods of Analysis.

Flame emission and atomic emission spectrometry. Theoretical principles, flame and flame temperature. Flame photometry; flame photometer, interferences, applications. Calibration curve method, effect of organic solvents, standard addition method and internal standardmethod. 4 hrs

Atomic Absorptin Spectrometry : Introduction, principle, advantages and limitations of AAS over flame emision spectrometry. Instrumentation, non-flame

techniques for atomization, vapour generation technique. Some typical applications of AAS ; oils, blood serum soils, ores, environmental samples.
4 hrs.

Fluorimetry : Introduction, flourescence and phosphorescence, factors affecting flourescence. Theory, relation between intensity of flourescence and concentration. Instrumentation and applications of Fluriometry.
2 hrs

Light scattering experiments, nephelometry, turbidmetry. Theory, instrumentation and applications. 2 hrs.

Mass Spectometry : Introduction, thoery, instrumentation . Methods of ionization ; electron impact (EI), arc and spark ionization , thermal ionization, chemical ionization, fast atom bombardment (FAB). Appearance potential, fragmentation patterns, molecualr weight determination, determination of molecular formula, isotope abaundances, measurement of ionization potential, miscellaneous applications. 5 hrs.

Thermal methods of analysis : Introduction, Thermogravimetry (TG) Differential thermal analysis(DTA), Differential Scanning Calorimetry(DSC). Instrumentation. Factors influencing results of TG and DTA . Applications of TG & DTA in the field of hydrates, minerals, inorganic and organic compounds, coordination compounds and analytical chemistry. Automatic thermogravimetric analysis. 5 hrs

Activation Analysis : Introduction, methods of analysis (Absolute and comparator methods) Limitations, advantages of analysis,applications of analysis. 2 hrs.

*Books Recommended*


1. Instrumental Methods of Analysis, H.W.Willard, L.L.Merrit, J.A.Dean and F.A.Settle
2. Introduction to Instrumental Analysis, R.D.Braun
3. Electroanalytical Chemistry, A.J.Bard
4. Electrochemical Techniques for inorganic Chemistry, J.B.Headridge.
5. Chromatography, Erich Heptaman
6. Standard Methods of Analysis Vol 3, F.J.Welcher.
7. Instrumental Methods of Analysis B.K.Sharma.
8. Instrumental Methods of Analysis, Chatwal and Anand
9. A hand book of instrumental Techniques for Analytical Chemistry, F.A. Settle (Ed)
10. Thermal Methods of Analysis, W.W.Wendlandt.
11. Fundamentals of Analytical Chemistry, 7th Edn, D.A.Skoog, D.M.West and F.J.Holler, Saunder College Publishing(1996).


CHI-4.2 : Nuclear Chemistry and Environmental Chemistry

1. Radioactive decay and equilibrium : Radioactivity, Rate of radio active process, methods determining half-lives, carbon dating, growth of radioactive products, radioactive equilibrium-transient and secular. 5 hrs.

2. Nuclear reactions : Q-value, coulomb barrier,cross-section, Bohr's theory of nuclear reactions, nuclear reactions brought about by n,p,d,t,e-electromagnetic radiation and heavy ions. Nuclear Reactions at high energies (spallation).
4 hrs.

3. Nuclear energy : Nuclear fission and fusion, Fission products and fission yields, types of reactors including Breeder reactor, nucler reactor and nuclear power

strategy in India, Nuclear fuel burn up factor, Nuclear fuels, Fusion as a potential source of energy, Principles and problems. 8 hrs.

4. Radioactive Techniques : Tracer techniques, labelled compounds aplications of isotopic tracers to chemical and biological problems, isotope dilution method, analytical applications neutron activation analysis, applications in industry, biology and medicine.

6 hrs.

5. Counting Techniques : GM, ionization and proportional counters. 2 hrs.

6. Radio toxictiy and nuclear waste management : Radio toxicity, biological effects of radiation, Design features of laboratories, maximum permissable dose limits, decontamination procedures and radioactive waste managements including waste storage and disposal procedures for institutional outside DAE.

5 hrs.

Environmental Chemistry.

1. Composition of the atmosphere, structure, Green house effect, air pollution, sampling and monitoring, acid rain, photochemical smog

4 hrs.

2. Water resources, water pollution, trace elements in water, monitoring techniques and methodolgy. Instrumental techniques in environmental chemical analysis, BOD,COD,

4 hrs.

3. Toxic chemicals in the environment, biochemical effects of As, Cd, Pb,Hg,CO,NOx, and SOx gases,Noise pollution. 4 hrs.

Environmental Toxicology :Chemical solution to environmental problems, biodegradability, principles of decomposition, better industrial processes.

8 hrs.

*Books Recommnded :*


1. Nuclear and Radiochemistry, G.Friedlander, J. Kennedy and J.M. Miller.
2. Source Book of Atomic Energy, S. Glasstone.
3. Introduction to Nuclear Physics and Chemistry, B.G. Harvey.
4. Essentials of Nuclear Chemistry, H.J. Arnikar.
5. Environmental Chemistry, S.E.Manahan, Lewis publishers.
6. Environmental Chemistry, A.K.De, Wiley Eastern
7. Environmental Pollution Analysis, S.M.Khopkar, Wiley Eastern.
8. Environmental Toxicity, Ed. J. Rose, Gordon & Beach Science Publication.


CHI-4.3 Organometallic Chemistry and Solid State Chemistry

Organometallic Chemistry :

Chemistry of Organometallic Compounds with pi-binding ligards: Synthesis, Structure and bonding in metal-carbon pi-bonded systems involving dihapto to hexahapto ligands viz., olefins, acetylenes, allylic moieties, butadienes, cyclobutadienes, cuclopentadienes and arenes. 10 hrs.

Fluxional behaviour of Organometallic Compounds.

1 hr

Homogeneous and heterogeneous catalysis involving metal complexes and organometallic complexes, oxidative additions, reductive elimination, insertion and deinsertion reactions, hydrogenation, hydroformylation, isomerisation, carboxylation, and polymerization, water gas shift reaction. 10 hrs.

Organometallic reagents in organic synthesis : organo iron, organo copper and organo palladium compounds.
2 hrs.

Solid State Chemistry :

Electrical properties : Survey of electrical properties and materials
1 hr

Superconductivity : Nature and properties of Superconducting materials, Meisner effect, Types I and II Superconductors, Theories, high temperature oxide Superconductors. Applications. 4 hrs

Ionic conductivity : Alkali halides; vacancy conduction. Silver chloride; interstitial conduction.

Solid electrolytes : (-Alumina, AgI and Ag+ion solid electrolytes. Anion conductors, requirements for ionic conductivity, Applications.
3hrs.

Conduction mechanism : Hall effect, Thomson effect, Peltier effect, Seeback effect. Thermocouples.

Dielectric materials, ferroelectricity, pyroelectricity, piezoelectricity. Applications of ferro-,pyro- and piezoelectrics. 3 hrs.

Magnetic Properties : Mechanism of ferro and antiferro magnetic

ordering, selected examples of magnetic materials, their structures and properties; metals and alloys, transition metal oxides, spinels, garnets, illemenites, pervoskites, magneto plumbites, applications, structure-property relation.
3 hrs.

Optical properties : Luminescence and phosphors, configurational coordinance model, some phosphor material, antistokes phosphors, lasers.
2 hrs.

Mechanical properties and dislocations in solids : Edge dislocations, screw dislocations, Structural transformation of solids : 2 hrs.

Solid solutions : Hume- Rothery rules, substitutional solid solutions and interstitial solid solutions. solid solution mecahnism, experimental methods for studying solid solutions (x-ray powder diffraction and density measurements ).
3 hrs

Alloy systems : Phase diagrams, two and three component systems, study of alloy systems; steels with reference to iron - carbon systems, copper-zinc system.
4 hrs.

Solid state reactions : Transitions, decomposition reactions, solid-solid reactions, photographic process. 3 hrs.

*Books Recommended*


1. Organometallic Chemistry : R .C. Mehrotra and A.Singh New Age International.
2. Principles of Organometallic Chemistry : G.E. Coates, M.L.H. Green, P.Powell & K.Wade.
3. Metallo-Organic Chemistry : A.J. Pearson, Wiley.
4. The organometallic Chemistry of the transition metals. R.H. Crabtree John. Wiley and sons.
5. Principles and Applications of organotransition metal chemistry J.P. Collman, L.S. Hegsdus, J.R. Nortan & R.G.Finks. University science books.
6. Inorganic Chemistry, 4th edition, J.E. Huheey, E.A. Keiter and R.C.Keiter. Addison-Wesley.

7. Advanced Inorganic Chemistry 6th Edn, F.A.Cotton, G.Wilkinson, C.A. Murillo & M. Bochman John-Wiley &sons.
8. Organometallic reagents in synthesis, P.R. Jenkins, Oxford Chemistry, Primer, Oxford University Press.
9. Solid state chemistry ; N.B. Hannay Prentice - Hall of India Pvt.Ltd. NewDelhi.
10. Solid state chemistry and its applications. A.R.West, John-Wiley & sons
11. New Direction in solid state chemistry, CNR Rao and J.Gopalkrishnan, Cambridge University Press.
12. Introduction to Solids, L.V. Azaroffs. McGraw Hill.
13. Principles of the solid state, H.V.Keer, Wiley Eastern.
14. Material Science and Engneering-a first course V.Raghavan, PrenticeHall of India Pvt Ltd.

CHI-4.4: Special topics in inorganic chemistry :

1. Non aqueous solvents

Importance of non aqueous solvents, typesof reactions, important reactons in liquid ammonia, anhydrous $H_2SO_4$, liquid $SO_2$, liquid $N_2O_4$,$BrF_3$, and fused salts. 9 hrs

2. Isopoly and heteropoly acids and their salts.

Niobate and tantalate isopolyanious, heteropoly niobates, isopoly and heteropoly acids and salts of molybdenum and tungsten. 5 hrs

3. Glasses, Ceramics, composites and nanomaterials.

Glassy state, Glass formers and glass modifies, applications. Ceramics strutures, mechanical properties, clay product,refractories, characterization, properties and applications.

Microscopic composites, dispersion-strengthened and particle reinforced,fibre-reinforced composites, macroscopic composites.

Nanocrystalline phase, preparations procedures, special properties and applications.
7 hrs

4. Analysis of materials

Analysis and characterization of common drugs, analegiscs, anti- psychotics, antihistamines, vitamins,sedatives, antibiotics and tranquilizers.
7 hrs.

5. Analysis of bewerages

Soft drinks, alcoholic drinks,tea,coffee, and fruit juice. 4 hrs.

6. Analysis of petroleum and coal

Proximate and ultimate analysis of coal. Analysis of petroleum products Kerosene,diesel and lubricant oils. 6 hrs.

7. Food analysis

Moisture,ash,crude protiens,fat,crude fibre, carbohydrates,calcium, potassium, sodium and phosphate. Food adulteration-common adulterrants in food, contaminationof food stuffs. Micrscopic examination and purification of sample HPLC, gas chromatography. Thin layer chromatography for identification of chlorinate

pesticides in food product.

12 hrs

*Books recommended*


1. Non aqueous solvents, H.Sisler
2. Non aqueous solvents, T.C.Wadington.
3. Advanced inorganic chemistry, (6thedn),F.A.Cotton, G.Wilkinson A.C.Murillo & M.Bochmann
4. Material science and engineering, An introduction -W.D.Callister, Wiley.
5. Principles of solid state-H.V.Keer, wiely Eastern.
6. Material science-J.C.Anderson, K.D.Leaver, J.M.Allexander, R.D.Rawlings,ELBS.
7. Principles of Instrument alanalysis- D.A.Sckoog, J.L.Loary, W.B.Saunders.
8. Basic concept of analytical chemistry-S.M.Khopkar, Wiley Eastern.
9. Hand book of instrumental technique for analytical chemistry- F.Settle, Prentice Hall.
10. Instrumental methods of analysis -Willard-Merritt,Dean and Settle.


CHI (Pr) 4.5 Lab Course in Inorganic Chemistry

a. Use of oxine, salicylaldoxime,DMG in the separation and estimation using volumetric/gravimetric method.

i) Cu + Ni, ii) Al + Mg

iii) Ni inpresence of Cr and Fe.

b. Analysis of ores
Hematite, Dolomite.

c) Analysis of alloy
Brass,Satinless steel, Cu-Nikel alloy.

Scheme of Examination Duration 7 hours

1. Volumetric gravimetric from a 35
2. Gravimetric/volumetric from (b or c) 35
3. Viva 05
4. Records 05

CHI (Pr) 4.6 Lab course in Inorganic Chemistry

1. Use of cation exchange resin
2. Use of anion exchange resin
3. Water analysis
4. Analysis of Fertiliser
5. Analysis of Food
6 Analysis of Cement
7 Use of Computer
8 Analysis of drugs
9 Iodine value
10 Use of Muffle Furnace
11 Use of AAS
12 Use of TLC
13 Use of Paper Chromatography
14 Extraction of organic compound from natural sources
i). Lycopene from tomatoes ii) B-Corotine from Carrots
15. Spectrophotometric estimation of Ascorbic acid, Aspirin and Caffeine
16. Semimicro Estimation of Nitrogen by Kjeldahl Method

Scheme of Examination Duration 7 hours

a). Experiment I (1-4) 35 marks
b). Experiment II (5-9) 35 marks
Viva 05
Records 05

*Books Recommended*

1. Vogel's Text Book of Quantitative Inorganic Analysis, J. Bassett, R.C.Denney, G.H.Jaffery and Mandham, Longmans, Green and Company Ltd.
2. Preparative Inorganic Chemistry, Brauer
3. Practical Inorganic Chemistry, G. Pass and H.Sutcliff, Chapman and Hall Ltd.(1968)
4. Standard Methods of Chemical Analysis- W.W.Scott and N.H.Furman.

## ORGANIC CHEMISTRY

CHO 4.1 : Retrosynthetic analysis, newer reagents, dyes and Natural products.

1. Startegy of organic synthesis.

Introduction to disconnection approach. Terminology:- Disconnection synthon, synthetic equivalent, Functional group interconversion (FGI) and target molecule (TM).

Application of retrosynthetic analysis to the following molecules :

Benzocaine, p-methoxyacetophenone, Saccharine, 1-cyclohexyl isopropenol, 1-phenyl-4-p-methxyphenyl-1,3-butadiene, Pirindol, 6-methylquinoline, veratrylamine, 3,5-dimethyl pyrazole, 2,4-dimethyl-3,5-dicarbethoxypyrrole, 4-methy l-2-aminothiazole, 2,3-dimethylindole. 10 hours.

2. Newer reagents in organic synthesis.

Use of the following reagents in organic synthesis and functional group transformations: DCC, 1,3-dithiane (reactivity and umpolung), LDA, DDQ, Wilkinson catalyst, $Bu_3SnH$, Baker's yeast. Prevost reaction, Woodward Prevost hydroxylation and phase transfer catalysts. 10 hours

3. Alkaloids : Detailed study of structure elucidation, stereochemistry, synthesis and biological uses of the following alkaloids.

Harmine, Harmaline, Yohimbine, Lysergic acid, Physostigmine. Biogenesis of alkaloids : Morphine, Harmine and Gramine. 10 hours.

4. Vitamins and Nucleic acids.

Vitamins-Structure, stereochemistry, synthesis and biochemical action of the following :

Vitamin H, Vitamins of E and K group.

Nucleic acids- classification, hydrolytic products of nucleic acids. Structure and synthesis of nucleosides, nucleotides and polynucleotides. Crick-Watson structure of DNA. Role of DNA in protein biosynthesis. Genetic code. 10 hours.

5. Dyes : Modern theories of colour and constitution. Classification of dyes.

Methods of Dyeing

Synthesis and application of the following dyes :

Acid azo dyes : Ponceau 2R; Napthol Blue Black 6B.

Basic azo dyes : Crysoidin G, Bismark Brown

Direct azo dyes : Congored, Rosanthrene O; Procin dyes : Ramazol Mordant azo dyes : Chromotrope 2B

Triphenylmethane dyes : Pararosanilineand crystal violet. Aurin, Chrome violet

Cyanine dyes : Classification, application in photography. Quinoline blue and sensitol red.

Fluorescent brightening agents, Tinopal B.V. 10 hours.

*Books Recommended*


1. Organic Synthesis - The Disconnection Approach by Stuart Warren.
2. Designing Organic Synthesis by Stuart Warren.
3. Modern Synthetic Organic Chemistry by H.O.House W.A.Benjamin INC, New York (1969).
4. Organic Chemistry Vol, II by I.L.Finar 6th Edition ELBS London (1998).
5. Steroids by Fieser and Fieser.
6. Chemistry of Vitamins by S.F.Dyke. Interscience London
7. Chemistry of Synthetic Dyes by K. Venkataraman. Academic Press, New York (1970).
8. Vitamins and Coenzymes by Wagner and Folkes.
9. Introduction to Nucleic acids by Harber, Domagle and Muller.


CHO 4.2 : Pharmaceutical chemistry, heterocycles and Organometallic compounds.

1. Medicinal chemistry -I

Drugs : Historical evolution of drugs. Theories of drug action. Classification. Metabolism of drugs. Mode of action, structure-activity relation (SAR) and synthesis of the following drugs.

Sulpha drugs : Cowel's ionisation and Kumler's resonance theories.

Sulphanilamide, Sulphadiazine, Sulphamethazine, Sulphaguanidine, Sulphamerazine, Sulphathiazole and sulphisoxazole.

Antimalarials : Chemotherapy of Malaria. 4-Aminoquinolines- Chloroquine.

8-Aminoquinoline-Pamaquine. Acridines- Quinacrin (Atebrin).

Guanidines-Paludrine (chlorguanide)..

Antifertility drugs ; Steroidal-Norethindrone, mestranol and Norgestrel. Non-steroidal, antifertility drugs. 10 hours

2. Medicinal chemistry - II

Mode of action, structure-activity relation (SAR) and synthesis of the following drugs :

Anticancer (antineoplastic) drugs : Nitrogen mustards :Chlorambucil, Sarcolysin, Dopan and Cyclophosphamide.

Pteridines : Amethopterin, Pyrimidines, 5-Fluorouracil.

Analgesics ; Classification- Narcotic and non-narcotic analgesics.

Narcotic analgesics-Opium alkaloids-Morphine and Codeine (Synthesis not necessary). Morphinans, Morphine, Metopan, Benzomorphan and phenazocine.

Non-narcotic analgesics :Aspirin. 4-phenylpiperidines-Pethidine, Diisopropylamines-Methadone. Pyrazolones-Antipyrine.

Antiviral drugs :- Amantidine, Rimantadine, Trometadine, Idoxuridine, Virolopic, Vidaraline, Acylclovir (Zovirox)and Zidovuadine (Retrovir). (Stuctures only) 10 hrs.

3. Heterocyclic compounds - II :

Seven membered heterocycles :- Azepines and benzodiazepines.

Ring transformations of heterocycles : Coumarin to benzofuran, Sydnone to Pyrazoles, Chromones to Pyrazoles, Furans to Pyridines, Pyrroles to Pyridines.

Heterocycles in functional group transformations :-

Alkanes from thiophenes, cycloalkanes from pyrazolines, Dienes from pyrroles, Alcohols from isoxazodiolines, esters from trichloroiscyanuric acid, Acetylenes from 1,2,3, selenadiazoles and deoxygenation of phenols with tetrazoles. 10 hours.

4. Antibiotics.

Structure, stereochemistry,synthesis and uses of the following antibiotics:

Natural pencillins and their commercial synthesis. Semisynthetic pencillins, Streptomycin, Chloramphenicol and patulin.

Tetracycline antibiotics :- Terramycin (structural elucidation only).

Structural features and uses of common antibiotic drugs-Norfloxacin

Rifamycin and Amoxycillin. 10 hours.

5. Organometallic compounds in organic synthesis :

Organoborane, Organolithium, Organosilicon and Organocopper compounds. 10 hours.

*Books Recommended*


1. Medicinal Chemistry by Alfred Burger. Vol-II Wiley-Interscience New York (1988).
2. Progress in Medicinal Chemistry Vol, 1-8. Edited by G.P.Ellis and G.B.West. North Holland, New York (1974).
3. Organic Chemistry Vol, I and II by I.L. Finar ELBS 6th Edition (1989)
4. Principles of Modern Heterocyclic Chemistry by Leo Paquette W.A. Benjamin, Inc, NY (1968)
5. Principles of Organometallic Chemistry by MLH Green, G.R.Caoter & R. W. H. Waddington.
6. An Introduction of the Chemistry of Heterocyclic Compounds, by R.M. Acheson. John Wiley and Sons 4th Edition.
7. Heterocyclic Chemistry by A.R.Katritzky and J.J.Logowski Methuen.
8. Heterocyclic Chemistry by T.Gilchrist, Butterworths London (1985).
9. Modern Heterocyclic Chemistry by Joule and Smith.


## CHO 4.3 : Pericyclic reactions, reaction mechanism, Photochemistry and Polymers

1. Reaction mechanism II.

Addition reactions:- Addition to carbon-carbon multiple bonds. Addition of carbon, Nitrogen, oxygen, and Sulphur nucleophiles to carbonyl group-Aldol reactions, Perkin, Stobbe, Dieckmann and Claisen ester condensation Electrophilic and Nucleophilic addition to C=C, C=O and conjugated systems-Michael addition.

Elimination reactions : E1, E2,E1CB mechanisms and orientations. Saytzeff and Holfmann rules. Elimination Vs Substitution. 10 hours.

2. Molecular Rearrangements

Carbon-carbon migrations-Dienone-Phenol, Benzilic acid, Favorskii, Neber, Sommelet-Hauser, Amadori,Stevens and Smiles

Carbon-nitrogen migration-Benzidine.

Carbon-oxygen-Baeyer-Villiger oxidation.

Oxygen-carbon-Fries.

3. Photochemistry :- Principles of Photochemistry-

Photochemistry of functional groups : Carbonyl compounds-n- * and - * transitions. Norrish type Iand II cleavages. Paterno-Buchi reaction.Photoreduction.

Enones- Hydrogen abstraction. Rearrangements of - -unsatured ketones, cyclohexadienones, p-Benzoquinones, Alkanes-Cis and transisomerisation. Benzene and its 1,2 -,1,3-and 1,4- additions.

Photosensitisation and phtoenolisation. 10 hours.

4. Dynamic Stereochemistry II- Pericyclic reactions, Introduction and classification.

Electrocyclic processes - Woodward Holfmann rules.

Cycloadditon reactions -Thermal and photochemical 2+2 and 4+2 cycloadditons. Correlation diagrams. Diels-Alder reactions. Sigmatropic rearrangements : Supra- and antarafacial H-Shifts. Claisen and Cope

re-arrangements. 10 hours

5. Polymers : Types of polymers.

Synthesis of polymers : (i). Addition or chain growth polymerisation-free radical and ionic vinyl polymerisation. (ii) Zeigler-Natta polymerisation. (iii) Condensational or step growth polymerisation. (iv) Co-polymerisation. Physical properties of polymers. study of polyesters, polyamides, phenol-formaldehyde resins, urea-formaldehyde resins and epoxy resins. Polyurethanes. 10 hours.

*Books Recommended*


1. Advanced Organic Chemistry-by Jerry March.
2. Comprehensive Organic Chemistry Vols I-IV-by Barton and Ollis.
3. Theory and mechanism in Organic Chemistry -by Lowry and Richardson.
4. Organic Chemistry Parts I & II by Carey and Sandberg.
5. Molecular Rearrngements - I and II P.de. Mayo.
6. Mechanisms of Molecular Migrations. Vol. I and II, by B.S. Thyagarajan, Wiley - Interscience, London 1st Edition. (1979).
7. Molecular Transformations in Organic Chemistry by D. Ranganathan and S. Ranganathan Macmillan India, New Delhi, 1st Edn. (1975).
8. Aromatic Character and Aromaticity by G.M. Badger Cambridge, University Press.
9. Molecular Photochemistry by N.J. Turro.
10. Molecular Reactions and Photochemistry by Depoy and Chapman.
11. Organic Photochemistry by J.M. Coxan and B.Halton, Cambridge University Press, London 1974.
12. A Text Book of Polymer Science by P.W. Billmeyer, John Wiley, Toppan.
13. Principles of Polymer Chemistry by P.J.Flory, Cornell University Press.
14. Natural and Synthetic High Polymers by K.H. Meyer, Interscience Publishers.
15. Polymer synthesis by Sandler and Kara Academic Press.
16. Preparative Methods of Polymer Chemistry by Sorenoson Campbell Interscience.


CHO 4.4 : Agrochemicals, natural products, pigments and Application of spectroscopic techniques.

1. Prostaglandins :

Introduction, nomenclature, classification and biological role of prostaglandins. Structural elucidation and stereochemistry of PGE1, PGE2, and PGE3. Total synthesis of PGE1 by Stork's, Corey's and Upjohn's approach. 10 hours.

2. Oils and Fats

Nomenclature and classification of fatty acids. Study of saturated, unsaturated, branched oxygenated and some having novel structures. Essential fatty acids, classical and modern methods of separation and isolation of fatty acids from oils and fats. Biosynthesis of fatty acids, Hydrogenation and autooxidation of oils and fats.
10 hours.

3. Agrochemicals and Pheromones.

Insecticides :- Fumigants and repellants.

Insecticides of plant origin-Nicotinoids, Pyrethroids and Rotenoids.

Synthetic organic insecticides- Nitrophenols. Halogen derivatives of hydrocarbons-DDT,DDD(TDE), methoxychlor, BHC and heptachlor.

Organophosphorus pesticides- Parathion, malathion and Chlorthion. Carbamic acid derivative-Baygon.

Pheromones : Origin and properties of insect sex attractants , synthesis and applications of Bombykol, a-multistriatin and 3,11-dimethy 1-2-nonacosanone.
10 hours

4. Natural porphyrins.

Chemistry of Haemoglobin and Chlorophyll. Organic pigments-Phthalocyanines.
10 hours

5. Application of spectroscopic methods in structural elucidation of organic molecules. Some examples from natural products viz terpenes alkaloids, steroids and antibiotics 10 hours.

*Books Recommended*


1. Prostaglandins by A.Mitra.
2. Industrial Oil and Products Vol-I by. Baileys.
3. Introduction to the Chemistry and Biochemistry of Fatty acids and thier Glycerides by F.D.Gunstone Chaoman & Hall 1980 (London).
4. Organic Chemistry Vol-II by I.L.Finar E.L.B.S. London (1990)
5. Comprehensive Organic Chemistry Vol, I-IV by barton & Oils Pugmon Press Oxford (1979)
6. Spectroscopic methods in Organic Chemistry by D.H. Williams & I.Fleming Mc. Graw-Hill, London (1989)
7. Organic Spectroscopy by D.W. Brown, A.J.Floyd, & M.Sainsburg, John Wiley &Sons, New York (1988).


CHO (Pr).- 4.5

Practical-I. Estimation of the following.

1) Nitrogen By Kjehldhal method
2) Nitro group By reduction
3) Hydroxy group by acetylation

Practical-II. Fractional distillation of Binary Liquid mixture.

CHO(Pr)-4.6

Preparation of Organic compounds involving multiple stages.

Scheme of Examination (Duration 7 hrs)

CHO (Pr)-4.5 Practical-I

Estimation 50 marks

Separation by Fractional Distillation/ TLC experiments20 marks

Viva 05 marks

| | |
|---|---|
| Journal | 05 marks |
| Total | 80 marks |

CHO (Pr).- 4.6 Practical-II

| | |
|---|---|
| Two/three stage preparation | 60 marks |
| Purification | 10 marks |
| Viva | 05 marks |
| Journal | 05 marks |
| Total | 80 marks |

*Books Recommended*

1). Vogel's Practical Organic chemistry edited by A.J.Hannaford & others. ELBS (London)1998.
2). A hand book of organic chemistry by H.T.Clarke.
3). A laboratory manual of organic chemistry by B. B. Dey. And T.R Govindachari.

## PHYSICAL CHEMISTRY

### CHP-4.1 : Chemical Bonding and Solid State Chemistry

#### Chemical Bonding

Molecular orbital and valence bond theories of chemical bonding, comparison of the two application to hydrogen molecule ion, $H_2$ molecule. Improvements in the Hitler-London wave functions, exchange symmetry of wave functions and the Pauli principle. Slater orbitals and SCF method for many electron atoms. Bonding and antibonding molecular orbitals. Molecular orbital theory applied to homonuclear and heteronuclear diatomic molecules.

13 hrs.

Polyatomic molecules : localized and non-localized molecular orbitals, hybrdization and direct valence. Conjugated and aromatic molociles ; Simple Huckel molecular orbital thoery and m.o.description of normal and cyclic butadienes, ethylene and aromatic molecules (benzene as an example). Calculation of delocalization energies, fractional bond orders, charge density calculations, extended Huckel theory and its simple chemical applications. 12 hrs.

#### Solid State Chemistry :

1. Different types of solids : Ionic, covalent, metallic, molecular and hydrogen bonded crystals. Lattice energy of ionic crystals. Theories of metallic state, properties of solids (only elementary account mechanical, thermal, magnetic electrical and optical)

8 hrs.

2. Defects in Solids : Frenkel and Schottry defects, line, surface and volumetric defects, kinetics of formation of defects in solids and chemical reactivity of solids.

5 hrs.

3. Semiconductors : Bonding and conductivity, mechanism of conductivity, energy bands in semiconductors, impurity conductors and p-n and n-p-n junctions. Importance of semiconductors. 6 hrs.

4. Super conductors : Occurance of super conductivity, its destruction by magnetic fields, microwave and I.R.Properties, isotope effect, B.C.S. theory of superconductivity, presistant currents. 6 hrs.

Total 50 hrs

*Books Recommended*


1. Quantum Mechanics -L.T.Schiff, Prentice-Hall.
2. Quantum Chemistry-H.Eyring.J.Walter and G.E.Kimball, John Wiley.
3. Quantum Mechanics- An introduction -H.L.Strauss, prentice Hall of India.
4. Quantum Mechanics- L.Pauling and E.B. Wilson, McGraw Hill.
5. Contemporary Quantum Chemistry-J.Goodisman, Plenum/Rosetta.
6. Quantum Chemistry-K.S.Pitzer, Prentice-Hall.
7. Introductory Quantum Mechanics- Valdimir Rojanstry.
8. Quantum Chemistry-John P.Lowe.
9. Physical Chemistry -P.W.Atkins, Claredon Press, Oxford 1970.
10. Molecular Quantum Mechanics-P.W.Atkins, Claredon Press, Oxford 1970
11. Introduction to Quantum Chemistry-J.M.Anderson.
12. Introduction to Quantum Mechanics-R.H.Dicke,J.P.Wittke.
13. Introductory Quantum Chemistry- A.K.Chandra Tata McGraw Hill, New Delhi,1994.
14. Quantum Mechanics in Chemistry-M.W.Hanna. The Benzamin/Cumming Publishing Co. Inc.
15. Quantum Chemistry-R.K.Prasad, New Age International Publishers New Delhi.
16. Solid State Chemistry-N.B.Hanna
17. Solid State Physics-A.J.Dekkar, Mac Millon, India Ltd.1993
18. Solid State Chemistry-C.N.R.Rao, Cambridge, CUP
19. Solid State Physics, Edited by R.Kube and Takeo Nagamiya McGraw Hill Book Co.Inc.
20. Introduction to Solids- L.V.Azaroff, McGraw Hill, New York.
21. Principles of Solid State Chemistry-A.R.West, John Wiley 1984
22. Principles of Physical Chemistry-R.M.Rosenberg, Oxford University Press.


CHP 4.2 : Statistical Mechanics, Statistical Thermodynamics, Catalysis, Reaction Dynamics, and Electrochemistry.

1. Statistical Mechanics and Statistical Thermodynamics

Microscope and Macroscopic systems.

Microstates and macrostates. Assemblies of independent localised and non-localised systems. Phase space or r-space and m-space. Ensembles.

2 hrs.

Classical Statistics

Maxwell-Boltzmann distribution for ideal gases and mixture of gases. Determination of Lagrangian multipliers, alpha and beta. Equipartition of energies. Maxwell-Boltzmann law of distribution of velocities and energies; average, root mean square and most probable velocities.

5 hrs.

Quantum Statistics :

Bose-Einstein, Fermi-Dirac and Maxwell-Boltzmann statistics and comparision between them

4 hrs.

Heat Capacities of Solids :

Einstein's theory of heat capacity of solids, Debye's theory. Characteristic temperature and use of Debye equation for the determination of heat capacity at

low temperature

5 hrs.

Partition Functions : Definition of partition function and separation of partition functions. Translational, rotational, vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules.

5 hrs.

Sackur - Tetrode equation : Entropies and heat capacities of ortho-, para-hydrogen systems, comparision of third law entropies with statistical entropies.

4 hrs.

2. Reaction Dynamics

absolute rate theory, potential energy surfaces, methods employed in the construction of potential energy surfaces, calculation of activation energy, relative rates: isotope effects.

5 hrs.

Effect of solvent, pressure and ionic strength for ion-ion, ion-neutral molecule type reactions, cage effects.

Fast reactions: flow methods, stopped flow technique, Relaxation methods and flash photolysis. 3 hrs.

3. Catalysis and Adsorption

General acid-base catalysis and specific acid-base catalysis : Bronsted relation and linear free energy changes, Zucker-Hammett hypothesis and Bunnett hypothesis.

Enzyme Catalysis :

Mechanism of single substrate reactions, Michaelis-Menten mechanism, influence of pH, temperature and inhibitors.

3 hrs.

4. Electrochemistry

Electrical double layer : Lippman equation, theories of electrical double layer-Helmholtz-Perrin, Gouy-Chapman and Stern theories. Effect of ions on zeta potential. Activity of ions in solution: ion-solvent interactions, ion-ion interactions and free energy of ions in solution. Born model and modifications, solvation number and their determination. Debye-Huckel and Bjerrum models and the corresponding theoretcal expression for activity coefficients, extension of the theory to higher concentration, triple ion formation and conductance minima.

8 hrs.

Total : 50 hrs.

*Books Recommended :*


1. Statistical Mechanics, N. Davidson, McGraw-Hill, 1962
2. Introduction to Statistical Thermodynamics, M. Dole, Prentice Hill. 1954
3. Statistical Thermodynamics, R.H. Fowler and E.A. Guggenheim,Cambridge University Press, 1939.
4. An Introduction to Statistical Mechanics, T.L. Hall, Addison Wesley, 1960.
5. Introduction to Statistical Mechanics, G.S. Rushbrook, Oxford University Press, 1949.
6. Statistical Mechanics, J.E. Mayer and M.G. Mayer, John Willey, 1940.
7. Catalysis by metals, G. C. Bond, Oxford, 1974.
8. Treatise on Physical Chemistry, H.S. Taylor and S. Glasstone Vol II, D. Van Nostrand, 1961.
9. Chemical Kinetics, K.J. Laidler. Mcgraw-Hill 1950.

10. Theory of rate processes, S. Glasstone, K.J. Laidler and H. Eyring Mcgraw-Hill 1941.
11. Kinetics and Mechanism, A Frost and R.G. Pearson, John Wiley, 1953.
12. The foundations of Chemical Kinetics, S.W. Benson, McGraw-Hill,1960.
13. Kinetics of Chemical Changes in Solution, E.S. Amis, McMillan, 1948.
14. The Kinetics of Chemical Change, C.N. Hinshelwood, Oxford, 1942.
15. Free Radical mechanisms, E.W.R. Steacies, Reinhold, 1946.
16. Techniques of Organic Chemistry, Weissberger (Ed) Vol VIII, Investigations of Rates and Mechanism of Reactions Interscience, 1963.
17. Theories of Chemical Reactions Rates, K.J. Laidler, Mcgraw-Hill, 1969.
18. Fast teactions D.N. Hague, Willey Interscience, N.Y., 1971.
19. The Principles of Electrochemistry, D.A. Mackinnes Reinhold, 1939.
20. Electrolyte Solutions, R.A. Robinson and R.H. Stokes, Academic, 1959.
21. Text Book of Electrochemistry, G.F.A. Kortum and J.O.M. Bockris, Elsevier, 1951.
22. Introduction to Electrochemistry, S. Glasstone, D. Van Nostrand, 1942.
23. Modern Electro Chemistry, J.O.M. Bockris and A.K.N. Reddy, Vol I and II, Plenum 1970.

## CHP 4.3. : Molecular Structure - II

### 1. Electron Spin Resonance Spectroscopy

Theortical principles and instrumentation. ESR spectra of hydrogen and nitrogen atoms, Semi-quinone ion, napthalene negative ion, methyl radical and methyl substituted radicals Zero field splitting ,Kramers degeneracy. Measurements of distribution of unpaired electrons in radicals. Study of co-ordination comppounds by ESR technique.

14 hrs.

### 2. Diffraction Studies

X-Ray Diffraction

Reciprocal lattice, indexing of single crystal rotation photographs, determination of molecular parameters, the geometric structure factor, Fourier series and the phase problems. Refinements of Fourier procedures. 10 hrs.

Neutron diffraction

Neutron diffraction and differences from X-Ray diffraction 2 hrs.

Electron diffraction

Theoretical principles structure analysis : Visual comparison of intensities, radial distribution function and its refinements. The rotating sector method.

4 hrs.

### 3. Symmetry properties of Molecules and group theory

Symmetry elements,Symmetry operations and point group. Determination of point group. Construction of group multiplication tables. Symmetry species and character tables. Reducible and irreducible representations. Analysis of reducible representations. Number of normal modes ofvibrational symmetry types. Rule of mutual exclusion. I.R.and raman active fundamentals.

20 hrs

Total 50 hrs.

*Books Recommended*

1) Physical Methods in Inorganic Chemistry-R.S. Drago East West Press, New Delhi

2) Molecular Spectroscopy-J.D.Graybreal, McGraw Hill
3) Spectroscopy, Vol.I,II and III-ed. Walker and Straughan, Chapman and hall London.
4) Chemical Applications of Group Theory -F.A.Cotton, Wiley Eastern, New Delhi
5) Molecular Symmetry -D.S.Schonlnd, Van Nostrand Comp.London,1965
6) Symmetry in Chemistry-Jeffe and Orchin, Wiley Inter Science, NewYork.
7) Symmetry, Orbitals and Spectra -Jeffe and Orchin, -Jeffe and Orchin, Wiley Inter Science, New York,1971.
8) Molecular Structure : A physical Approach-J.C.D.Brand and J.C. Speakman, Edward Arnold Ltd. London
9) Spectroscopy and Molecular Structure-G.W.King
10) Electron Diffraction- T.B. Rymer, Methuen, London,1970
11) Neutron Diffraction - G.E.Becon
12) Symmetry in Molecules-J.M.Hollar
13) X-Ray Crystallography-Buerger
14)Diffraction Methods- Wernard
15) Chemical Crystallography-L.W.Bunn. N.Y.and Oxford,1945
16) Crystals and X-Rays K.landsdale, N.Y.1945
17) Crystal Structure Analysis- M.J.Berger, john Wiley and sons, N.Y.1960
18) The Determination of Molecular Structure- P.J.Wheatley, Clarendon ,Oxford,1960
19) Physical Chemistry-G.M.Barrow, McGraw Hill, New York, 1991
20) X-ray Diffraction - D.B.Cullity, Mass Addison, Wesley,1978.
21) Introduction to Molecular Spectroscopy - G.M.Barrow, McGraw Hill, New York, 1985
22) Group Theory in Chemistry- V.Ramakrishnan and M.S.Gopinathan,Vishal Publishers, Jalandhar,1988.

CHP 4.4 : Molecular Structure III

1. Raman Spectroscopy :

Theortical principles and instrumentation. ESR spectra of hydrogen and nitrogen atoms, Semi-quinone ion, napthalene negative ion, methyl radical and methyl substituted radicals Zero field splitting ,Kramers degeneracy. Measurements of distribution of unpaired electrons in radicals. Study of co-ordination comppounds by ESR technique.

14 hrs.

2. Diffraction Studies

X-Ray Diffraction

Reciprocal lattice, indexing of single crystal rotation photographs, determination of molecular parameters, the geometric structure factor, Fourier series and the phase problems. Refinements of Fourier procedures. 10 hrs.

Neutron diffraction

Neutron diffraction and differneces from X-Ray diffraction 2 hrs.

Electron diffraction

Therotical principles structure analysis : Visual comparison of intensities, radial distribution function and its refinements. The rotating sector method.

4 hrs.

3. Symmetry properties of Molecules and group theroy

Symmetry elements,Symmetry operations and point group. Detrmination of point group. Construction of group multiplication tables. Symmetry species and character tables. Reducible and irreducible representations. Analysis of reducible

representations. Number of normal modes of vibrational symmetry types. Rule of mutual exclusion. I.R.and raman active fundamentals. 20 hrs

Total 50 hrs.

*Books Recommended*


1) Physical Methods in Inorganic Chemistry-R.S. Drago East West Press, New Delhi
2) Molecular Spectroscopy-J.D.Graybreal, McGraw Hill
3) Spectroscopy, Vol.I,II and IIIed. Walker and Straughan, Chapman and hall London.
4) Chemical Applications of Group Theory -F.A.Cotton, Wiley Eastern, New Delhi
5) Molecular Symmetry -D.S.Schoneled, Van Nostrand Comp.London, 1965
6) Symmetry in Chemistry-Jeffe and Orchin, WileyInter Science, New York.
7) Symmetry, Orbitals and Spectra -Jeffe and Orchin, -Jeffe and Orchin, Wiley Inter Science, New York,1971.
8) Molecular Structure : A physical Approach-J.C.D.Brand and J.C.Speakman, Edward Arnold Ltd. London
9) Spectroscopy and Molecular Structure-G.W.King
10) Electron Diffraction- T.B. Ryner, Methuen, London,1970
11) Neutron Diffraction - G.E.Becon
12) Symmetrym in Molecules-J.M.Hollar
13) X-Ray Crystallography-Buerger
14) Diffraction Methods- Wernard
15) Chemical Crystallography-L.W.Bunn. N.Y.and Oxford,1945
16) Crystals and X-Rays K.landsdale, N.Y.1945
17) Crystal Structure Analysis- M.J.Berger, john Wiley and sons, N.Y. 1960
18) The Determination of Molecualr Structure- P.J.Wheatley, Claredon Oxford,1960
19) Physical Chemistry-G.M.Barrow, McGraw Hill, New York, 1991
20) X-ray Diffraction - D.B.Cullity, Mass Addison, Wesely,1978.
21) Introduction to Molecular Spectroscopy - G.M.Barrow, McGraw Hill New York, 1985
22) Group Theory in Chemistry- V.Ramakrishnan and M.S. Gopinathan, Vishal Publishers, Jalandhar, 1988.


## CHP 4.4 : Molecular Structure - III

### 1. Raman Spectroscopy :

Theories of raman effect, Concept of polarizibility and polarizibility ellipsoid. Vibrational Raman Spetcra, Rotational raman Spectra of Molecules. Symmetry selection rule and prohibition of inter combination. Influence of nuclear spin in case of homonuclear diatomic molecules. Rotational -Vibrational raman Spectra, principle of mutual exclusion, polarization of Raman lines and ortho- and para- modifications.

An introduction to laser resonance Raman spectroscopy. Elucidation of structure of molecules, e.g.$H_2O$, $NO_2$, $CO_2$ by Raman Spectra. 12 hrs

### 2. Photoelectron Spectroscopy :

Valence and binding energies, shift in energies due to chemical effects and Augar transitions. Instrumentation. Applications to free molecules and surfaces.
6 hrs.

### 3. Mossbauer Spectroscopy:

Principles, instrumentation,resonance line shifts, chemical shifts, quadrupole interactions and magnetic interactions. Applications of Mossbauer Spectroscopy.
6 hrs

4. Mass Spectrometry:

Instrumentation and theoretical principles, determination of empirical formula, fragmentation patterns and correlation with structure. Appearance potentials and ionization potential. 6 hrs

5. The Electric Properties of Molecules :

Electric dipole moment of molecules, polarization of a dielectric, polarizability of molecule. Clausius-Mosotti equation. Debye equation. Limitations of Debye theory. determination of dipole moment from dielectric measurements in pure liquids and solutions. Dipole moment and ionic character, Bond Moment, group moment, vector addition of momenta, bond angles. The energies due to dipole-dipole, dipole-induced dipole and induced dipole-induced dipole interactions. Lennard-Jones potential.

10 hrs.

6. The Magnetic Properties of Molecules :

Diamagnetism and paramagnetism. Volume and mass susceptibilities, Langevins classical theory of diamagnetism and paramagnetism. Atomic and ionic susceptibility. Pascal constants. Curie- weiss law. Van Vieck's general equation of magnetic susceptibility. Determination of magnetic susceptibility. Ferro-and antiferro magnetism. Applications to coordination complexes and complex ions of transition metals. 10 hrs

Total : 50 hrs.

*Books Recommended*


1. Introduction to Molecular spectroscopy, G.M.Barrow, McGraw Hill, New York.
2. Physical Methods in Inorganic Chemistry - R.S.Drago, East-West Press, New Delhi
3. Molecular Spectroscopy - J.D.Graybeal, McGraw Hill.
4. Spectroscopy, Vol.I,II and III. Ed. Walker and Straughan, Chapman Hall, 1976.
5. Infrared and Raman Spectra of Polyatomic Molecules - G.Hertzberg, Van Nostrand, New York, 1954.
6. Absorption Spectroscopy, R.P.Bauman, Wiley New York,1952.
7. Introduction to Photoelectron Spectroscopy - P.K.Ghosh., John Wiley
8. Photoelectron Spectroscopy - T.H.D. Eland. Butterworth, London, 1974.
9. Fundamentals of Molecular spectroscopy, C.N.Bawell, Tata McGraw Hill, New York,1985.
10. Magneto chemistry - P.Selwood , Interscience, New York, 1956.
11. Techniques in Organic Chemistry, Vol.I.Interscience, 1963
12. Mass Spectroscopy : organic Applications, K.Beiman, McGraw Hill.
13. Introduction to Mass spectroscopy and its Applications-R.W.Kiser,
14. Prentice Hall, Englewood-Cliff (NJ) 1965.
15. Basic Principle of Spectroscopy - Raymond Chang, McGraw Hill Kogakusha Tokyo,1971.
16. Physical Chemistry G.M.Barrow- McGraw Hill, New York, 1991.
17. Instrumental Methods of Analysis- Willard, Merit and Dean, TatMagraw Hill, New Delhi, 1993.
18. Molecular Interpretation of Mass Spectroscopy, F.W.Mclafferty and W.A.Benzamin.
19. Molecular Spectroscopy -I.N.Levin, Interscience.
20. Electron Spin Resonance, Elementary Theory and Practical Applications, J.E.Wetz and Boulton -McGraw Hill.
21. Introduction to Magneto Chemistry -E.L.Ernshaw, Academic Press.

22. Electrical and Optical Properties of Molecular behaviour -M.davies, Pergoman Press.
23. Polar Molecules -P. Degye, Dover Publications.

CHP (Pr) -4.5: Lab. Course in Physical Chemistry.

1) Viscocity
   Determination of molecular radius of glycerol by viscocity measurements.
2) Surface Tension
   a) Comparison of cleansing powers of two detergent samples.
   b) Comparison of a mixture of two liquids
3) Solubility Variation of solubility of Ca(OH)2 in NaOH solution and hence determination of the solubility product of Ca (OH)2.
4) Phase Equilibria
   a) Phase diagram of napthalene and diphenyl system.
   b) Phase diagram of acetamide and salicylic acid or picric acid and benzene.
5) Thermochemistry
   a) Heats of neutralisation of HCl and $CH_3COOH$ and thier relative strength.
   b) Heat of reaction (precipitation/formation) of $BaSO_4$.
   c) Heat of transition of Glauber's salt ($Na_2SO_4.10H_2O$)
6) Refractometry
   Comparison of Mixture of unknown composition (including the case of salt solution)
7) Absorptiometry
   a) Dissociation constant of a weak acid
   b) Absorptiometric titrations of Fe(II) with $KMno_4$
8) Electrolytic Conductance
   a) Conductometric titrations :acid mixtures Vs NaOH
   i) Acetic acid + hydrochloric acid mixture Vs NaOH
   ii) Oxalic acid + hydrochloric acid mixture Vs NaOH
   iii) Acetic acid + Oxalic acid mixture Vs NaOH
   iv) Nitric and Sulphuric acid mixture Vs NaOH
   b) Conductometric titrations : Sodium acetate (or oxalate Vs NaOH
   c) Conductometric titrations : $HCl+NH_4Cl$ Vs NaOH
   d) Conductometric titrations : $H_2SO_4+CH_3COOH+CuSO_4$ Vs NaOH
9) Reaction Kinetics
   a) Decomposition of $H_2O_2$ catalysed by iodide ions.
   b) Iodination of acetone
   c) Study of Kinetics of hydrolysis of tertiary buty halide
10) EMF of Cells
   a) Heat of reaction and Ke of the reaction between metallic zinc and $pb(NO_3)_2$ Solution
   b) Estimation of halides in a mixture
   c) Titration of $HCl+CH_3COOH$ with NaOH

*Books Recommended*

1. Findlay's Practical Physical chemistry, 9th edition, revised by B.P. Levitt.
2. Practical Physical Chemistry by A.M.James and F.E.Prichard
3. Experiments in Physical Chemistry by Shoemaker and garland
4. Experiments in Physical Chemistry by Daniels, Alberty and Williams et.al.
5. Laboratory Physical Chemistry by Oelke / M.A.C.T.L.A.C.

6. Experiments in Physical Chemistry by W.G.Palmer
7. Advanced Physico-Chemical experiments by J.Rose
8. Experimental Physical Chemistry by V.D.Athwale and Paul Mathur , New Age International Publishers.
9. Text Book of Physical Chemistry by S.Glasstone
10. Text Books of quantitative analysis by A.I.Vogel
11. Advanced Practical Physical Chemistry by J.B.Yadhav, Goel Publishing House, Meerut.

Scheme of Examination (Short Exercise)

CHP (Pr)-4.5

Duration of examination_____ 7hours

a) Experiment I_____ 35marks

b) Experiment II_____ 35marks

c) Viva _____ 05 marks

d) Journal_____ 05 marks

CHP (Pr)-4.6 : Lab. Course in Physical Chemistry

1) Viscocity
   Effect of temperature on the viscocity of the liquid.
2) Surface Tension
   Molecular surface energy and association factor.
3) Solubility
   a) Variation of solubility of potassium hydrogen tartarate with ionic strength involving a common ion and determination of mean ionic activity coefficients.
   b) Influence of ionic strength on the solubility of CaSO4 and determination of its thermodynamic solubility product and mean ionic activity.
4) Phase Equilibria
   a) Formula of the complex formed between copper ions and ammonia by distribution method.
   b) Phase diagram of a three component system: water,benzene and ethanol or acetic acid, water and chloroform or benzene.
5) Thermochemistry Stepwise heat of neutralization of polybasic acid
6) Polarimetry Kinetics of inversion of sucrose and determination of catalytic coefficint.
7) Refractometry Molar refraction of a solid substance by dissolving it in a solvent.
8) Absorptiometry
   a) Investigation of complex formation of absorptiometry (e.g. Fe ( III ) salicylic acid, formula, stability constant, free energy and pH effects Fe (III)-sulfosalicylic acid and Ni-1,10-Phenanthroline).
   b) Composition of Cu(II)and Fe(III) solution by photometric titration with EDTA
   c) Ionization constant of bromphenol blue.
9) Electrolytic conductance Equivalent conductance of a weak electrolyte (e.g.acetic acid, formic
   acid)using Kohlrausch's law
10) Mobilities of ionsDetermination of the ionic conductance of Cu2+at infinte dilution by Hittorff's method.Reaction Kindetics
   a) Saponification of ethylacetate by titration method and conductometric method.
   b) Chromic acid oxidation of 2-propanol and determination of i) order ii) effect of addition of Mn(II) iii) effect of adding oxalic acid iv) test for chromium interversion v) substituent effects.
      oxidation of benzyl alcohols.
   c) Decomposition of oxalic acid in solution photosensitized by uranyl sulphate.
12) EMF of cells
   a) Stability of the complex $Ag(NH_3)_2$ (concentration cells)
   b) transport number of Ag+ and $NO_3$-in solution (concentration cells)
   c) Determination of the molecular state and the given calculation of the association/dissociation constant of the given solute

d) Determination of Hammet constant of ortho-, meta- and para amino/nitro benzoic acid by pH measurements.

13) Cryoscopy A study of complex formation between mercury and potassium halides.

*Books Recommended*


1. Findlay's Practical Physical Chemistry, 9th edition, revised by B.P.Levitt.
2. Practical Physical Chemistry by A.M.James and F.E.Prichard
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9. Text book of Physical Chemistry- by S.Glasstone
10. Text book of quntitative analysis- by A.I.Vogel
11. Advanced Practical Physical Chemistry -by J.B.Yadhav, GoelPublishing House, Meerut.


Scheme of Examination (Long Exercise)

CHP (Pr) - 4.6

Duration of examination.....7 hours

a) Experiment.....70 Marks

b) Viva.....05 Marks

c) Journal.....05 Marks