

**M.Sc. Semester I**  
**Course CHE2101**  
**Inorganic Chemistry-1 [3credits]**

**Unit I**

*Fundamentals of Quantum mechanics:*

Postulates of quantum mechanics, interpretation of wave function, properties of wave function, hermitian operators, expectation energy and mean value theorem. Particle in a box, quantum mechanical tunneling, quantum well, degeneracy of energy levels H-atom wave function, separation of translational and rotational parts of the Schrödinger equation, separation of radial and angular equations, solution of  $R(r)$ ,  $\Theta(\theta)$ ,  $\Phi(\phi)$  equations. Quantum numbers and their significance, shapes of the orbitals, energy of H-atom orbitals.

**Unit II**

*Quantum mechanics and multielectronic atoms:*

Multielectronic atoms, wave functions, Self Consistent Field, Hartree-Fock method. Energy levels in multielectronic atoms and ground spectral states. Spectral states of polyelectronic atoms, LS and jj couplings, allowed microstates of d electrons and spectral states. Racah and Slater parameters and their relationship with energies of spectral states, Zeeman and Stark effects. Spectra of alkaline earth metal ions. Electrostatic concept of complex formation, effect of ligand field geometry on the energy of d-orbitals, factors affecting crystal field splitting, spectrochemical series, Jahn -Teller Theorem.

**Unit III**

*Metal-Ligand equilibria:*

Metal - ligand equilibria in solution, stepwise and overall formation constants and their interpretation, trends in stepwise formation constants. Factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and macrocyclic effect. Determination of stoichiometry of complex formation, Determination of binary formation constants of complexes by pH - metry and spectrophotometry. Stability of mixed ligand complexes, astatistical stabilization, ring-size effect, inter ligand electron delocalization, intramolecular inter ligand interactions and their effect on the stability of ternary complexes.

**Books Recommended :**

1. Theoretical Inorganic Chemistry, M. C. Day and J. Selbin, Van Nostrand-Reinhold
2. Electron and Chemical bonding, H.B. Gray Benjamin, New York
3. Atomic Structure and Chemical Bonding , Manas Chanda McGraw Hill, New Delhi
4. Introduction to Atomic and Molecular Structure, J. Bartlet, John-Wiley & Sons, New York
5. The Chemical Bond , J. N. Murrell, S. F. A. Kettle and J. M. Tedder, John Wiley, London
6. Advanced Inorganic Chemistry , F. A. Cotton and G. Wilkinson, Wiley, London
7. Coordination Chemistry, Martell and Kelvin , Academic Press.
8. Coordination Chemistry, D. Banerjea, Tata McGraw Hill
9. Advanced Inorganic Chemistry, Series Vol.1-10, A.G.Sharp, Academic press
10. Inorganic Chemistry, J. E. Huhey, Harper International SI Edition.

.....

## Course CHE2102

### Organic Chemistry-1 [3credits]

#### Unit I

*Aliphatic nucleophilic substitution reactions:* The  $S_N1$ ,  $S_N2$ , and  $S_Ni$  reactions, their mechanisms and stereochemistry, leaving group effect and reaction medium, ambident nucleophile, Neighboring group participation (anchimeric assistance), Aliphatic electrophilic substitution reactions  $SE1$ ,  $SE2$  and  $SEi$  reactions, their mechanism and stereochemistry. Aliphatic addition reactions, electrophilic and nucleophilic addition reactions, mechanism, stereochemistry of additions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity, addition to cyclopropane ring.

#### Unit II

*Organic reaction mechanisms:* Mechanism, Types of reactions, thermodynamic and kinetic requirements, Potential energy diagram. Energy of activation, Transition state & intermediate, methods of determining mechanism, primary and secondary isotope effects, solvent effects, substituent effects. Effect of structure on reactivity, Hammett equation, linear free energy relationship. Substituent constant, reaction constant, correlation of change in reaction constant with mechanism, Taft equation.

#### Unit III

*Molecular rearrangements:*

Mechanism to nucleophilic, electrophilic, and free radical molecular rearrangements. Carbon-carbon rearrangements: Wagner-Meerwein, Tiffeneau-Demyanov, Favorskii, Wolff, Benzil-Benzilic acid, Neber, Benzidine rearrangements, Carbon-nitrogen rearrangements: Hoffmann, Curtius, Lossen Schmidt and Beckmann rearrangements. Carbon-oxygen rearrangements: Bayer-Villiger, Dakin and Wittig rearrangements.

#### Books Recommended:

1. Advanced Organic Chemistry, Jerry March
2. Physical Organic Chemistry, Jack Hine
3. Organic Chemistry, Stanley H. Pine
4. The Modern Structural Theory of Organic Chemistry, L.N. Ferguson
5. Comprehensive Organic Chemistry -D. H. R. Barton Vols.1-6
6. Organic Chemistry -R.T. Morrison and R. N. Boyd, 6th Edition
7. Guidebook to Mechanisms in Organic Chemistry, P. Sykes
8. Synthetic Approaches in Organic Chemistry, R. K. Bansal
9. Reaction Mechanisms in Organic Chemistry, S. M. Mukherjee and S. P. Singh
10. Understanding Organic Reaction Mechanisms, Adam Jacobs
11. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parashar, Narosa. 2002
12. Vogel's Textbook of Practical Organic Chemistry, Revised by B. S. Furniss, A. J. Hannaford, P.W.G. Smith, A. R. Tatchel.

.....

## Course CHE2103

### Physical Chemistry-1 [3credits]

#### Unit I

*Kinetic Theory of Gases:* Derivation of Maxwell's distribution law for molecular velocity and its applications in calculating molecular speeds: Most probable, average and root mean square. Intermolecular collisions, frequency of collision, Molecular collision and mean free path. Collision theory of reaction rates. Transport process: Thermal conductivity, kinetic theory of thermal conductivity of gases, viscosity, flow rate of fluids, measurement of viscosity of gases, relation between viscosity and mean free path of gases, effect of temperature on viscosity of gas. Diffusion of gases.

#### Unit II

*Chemical Kinetics :* Recapitulation. Complex Reactions : Reactions approaching equilibrium, steady state approximation, Rate laws for consecutive, opposing and parallel reactions, explosive reactions. Techniques to study gas phase reactions. Fast reactions; relaxation, stop flow and flash photolysis. Kinetics of enzyme reactions. Harpoon mechanism (Molecular Beam method). Activated complex theory: Reaction coordinate and the transition state, potential energy surface, concentration of activated complex and rate constant, experimental observation of activated complex. Thermodynamic aspect. Theories of unimolecular reactions: Lindemann and Hinshelwood. Third order reaction

#### Unit III

*Surfactants and solution behaviour:* Introduction of liquid surfaces and source of surface tension/interfacial tension. Methods of surface tension measurement Classification of surfactants, micellization, factors influencing CMC. Thermodynamics of micellization. Aggregation number and its determination, micellar solubilization, micro emulsion, reverse micelles, applications of various surfactant organized assemblies

#### Books Recommended:

1. Laidler, K. J., (1987) *Chemical Kinetics*, Third Edition, Pearson Education, Noida (India)
2. Levine, R.D., *Molecular reaction Dynamics*, (2009), Cambridge University Press, NY. (Paperback Edition)
3. Raja Ram J. and Kuriacose J.C., (1993). *Kinetics and Mechanism of Chemical Transformations*, MacMillan Indian Ltd., New Delhi
4. Rakshit, P. C., (2004) *Physical Chemistry*, Seventh Edition, Sarat Book Distributors, Kolkata
5. Moroi, V., *Micelles: Theoretical and Applied Aspects*, Plenum Publishers, New York.
6. Rosen, M.J. (1989) *Surfactants and Interfacial Phenomena*, Wiley, New York.
7. Levine, I.N., (2002) *Physical Chemistry*, Fifth Edition, Tata McGraw Hill Pub.Co. Ltd., New Delhi.
8. Engel, T. and Reid, P., (2007) *Physical Chemistry*, First Edition, Pearson Education, Noida
9. Ball, D. W., (2003) *Physical Chemistry*, India Edition Thomson Learning, USA
10. Atkins P. and De Paula J., (2006) *Atkins' Physical Chemistry*, Eighth Edition, Oxford University Press, New York.

## Course CHE2104 Analytical Chemistry-I [3 credits]

### Unit I Basics of Electroanalytical and Chromatographic Techniques

a) *Electrochemical methods:* Definitions and terminology involved in electrochemistry. *Specific ion selective electrodes:* Glass electrode for  $H^+$  /  $Na^+$  ions, solid membrane electrode for fluoride, liquid membrane electrode for calcium. Enzyme - substrate electrode for  $NH_3$ , and gas sensing electrodes for  $SO_2$ /  $NH_3/CO_2$  /  $O_2$ . Introduction to Amperometry and Non - aqueous titrations.

b) *Chromatography:* Column theory (qualitative approach), mechanism of separation and applications of adsorption, partition, ion exchange, affinity and size exclusion chromatography. Qualitative and quantitative analysis by chromatography

### Unit-II GC and HPLC

Introduction to Gas Chromatography: Instrumentation, types of columns, injection systems and detectors. Capillary GC, GCMS. Introduction to super critical fluid chromatography (SFC).

*Liquid Chromatography:* Principles, solvent delivery systems, injections system, detectors and columns. Size-exclusion chromatography.

### Unit III Thermal methods:

*Thermogravimetry analysis:* Principle, construction and working of thermobalance, factors affecting TGA, Applications of TGA.

*Differential thermal analysis and differential scanning calorimetry:* Principle, Instrumentation, factors affecting analysis and applications. Thermo mechanical analysis [TMA] Instrumentation and application, thermometric titrations.

### Books Recommended:

1. An Introduction to separation science, L.R. Snyder and C. Horvath, Wiley Interscience
2. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman 5<sup>th</sup> edition (1998), Saunders College Publishing, Harcourt Brace & Company, U.S.A
3. Electrochemical Methods: Fundamentals and Applications, A.J. Bard and L.R. Faulkner 2<sup>nd</sup> Edition (2000), Wiley, New York.
4. Fundamentals of Electroanalytical Chemistry, P Monk, John Wiley, NY.
5. Instrumental Analysis , Y.H. Bauer, G.D. Christian, S.E. O'reilly, Allyn and Bacon Inc.
6. Introduction to Thermogravimetric Analysis, C.J. Keattch and D. Dollimore.
7. Working with Ion selective Electrodes, O.K. Camman.

.....

## Course CHE2105 Spectroscopy-I [4 credits]

### Unit I(15h)

*Symmetry and Group theory:* Symmetry elements and operations, representation of symmetry operations as matrices, definition of groups, sets of symmetry operations of molecules satisfying the conditions of a group, generators. Axial, non-axial and special point groups.

### Unit II(15h)

Classes of operations, reducible and irreducible representations. Great orthogonality theorem, Derivation of character tables of  $C_{2v}$  and  $C_{3v}$  point groups. Projection operators and direct products. Transformation properties of atomic orbitals.

### Unit III(15h)

*NMR Spectroscopy:* Nuclear spin, nuclear resonance, saturation, relaxation, Basic instrumentation shielding and deshielding of magnetic nuclei, coupling constant, chemical shift and its measurements. Factors affecting chemical shift, spin - spin interactions and spin decoupling, Introduction to  $^{13}\text{C}$  - NMR and FTNMR

*Electron Spin Resonance :* Introduction, Instrumentation, electronic spin states in 1 and 2 electron systems, fine structure, applications.

### Unit IV(15h)

*X-ray Diffraction :* Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density.

*Electron diffraction :* Theory, measurement techniques and elucidation of structure of simple molecules. Low energy electron diffraction.

*Neutron diffraction:* Scattering of neutrons by solids & liquids. Measurement techniques, Elucidation of magnetically ordered unit cell.

### Books Recommended :

1. Physical Methods in Chemistry : R.S. Drago, Saunders College
2. Chemical applications of Group Theory , F. A. Cotton Wiley-Eastern, New Delhi
3. Symmetry in Chemistry, H. H. Jaffe and M. Orchin Wiley, New York
4. Group Theory and its Chemical Applications , P.K. Bhattacharya, Himalaya, New Delhi
5. Molecular Symmetry and Group Theory, R.L. Carter, Wiley
6. X- Ray methods : Clive Whiston, John Wiley & Sons.
7. Solid State Chemistry and its Applications, A.R. West, John Wiley & Sons, New York (1984)
8. Instrumental Analysis, D. A. Skoog, F.J. Holler and S.R. Crouch, Thomson Brooks/Cole, Cengage Learning, UK
9. Molecular Structure and Spectroscopy - G. Aruldas, Prentice Hall of India

.....

**M.Sc. Semester II**  
**Course CHE2201**  
**Inorganic Chemistry-II [3credits]**

**Unit I(15h)**

Chemical Bonding: Variation and linear combination principles, valence bond and molecular orbital interpretations of  $H_2^+$  and  $H_2$  molecules. Valence bond and molecular orbital interpretation of other diatomic molecules. Stability, bond energy and bond distance, Resonance concept. Directed valency: Pauling - Slater's concept.

Valence bond theory: Formation of hybrid orbitals, their wave functions and properties. Symmetry, composition of hybrid orbitals in and formation of linear  $AB_2$ , triangular  $AB_3$ ,  $AB_4$ ,  $AB_5$  and  $AB_6$  molecules.

Molecular Orbital Theory: Symmetry adapted linear combinations of terminal atom orbitals and formation of molecular orbitals in simple polyatomic compounds with triangular, tetrahedral and square planar geometry.

**Unit II(15h)**

Molecular geometry: VSEPR theory. Walsh diagrams. M-M multiple bonds. Structure and bonding in the metal complexes with p -acids, on the basis of spectral evidence. Stabilization of unusual oxidation states. Synthesis, structure and bonding in metal carbonyls and nitrosyls. M-M bonds in metal clusters. Cluster valence electrons and Wade-Mingos-Lauher rules. Structure elucidation based on CVE and spectroscopic data. Isolobal analogies. Applications of metal clusters.

**Unit III(15h)**

Multicentric boranes and their topology, carboranes and metallo carboranes. Inorganic Polymers and Ring compounds: Linear and cyclic Borazenes, phosphazenes and thiazenes. Phosphonitrilic polymers. Synthesis, structure and bonding in organoboron, organosilicon, organo phosphorous and organotin compounds. Applications of these compounds in organic synthesis.

**Reference Books:**

1. Lee J.D., (1991) Concise Inorganic Chemistry, 4<sup>th</sup> Edition, Chapman and Hall,
2. Puri B.R., Sharma L.R. and Kalia K.C., (2006). Principles of Inorganic Chemistry, 29<sup>th</sup> Edition, Milestone Publ., Delhi
3. Cotton F.A. and Wilkinson G., (2009) Basic Principles of Inorganic Chemistry, 3<sup>rd</sup> Edition, Wiley Eastern,
4. Mahan B.H., (2009) University Chemistry, 3<sup>rd</sup> Edition, Narosa Publ House, New Delhi.
5. Gilreath E. S., (1985) Fundamental Concepts of Inorganic Chemistry, 2<sup>nd</sup> Edition, McGraw Hill Int.

.....

## Course CHE2202

### Organic Chemistry-II [3credits]

#### Unit I

*Aromaticity:* Aromaticity and Huckel's rule, Aromaticity in benzenoid and non-benzenoid compounds, annulenes, fullerenes. Alternant and non-alternant hydrocarbons, energy level of molecular orbitals, antiaromaticity, homoaromaticity, non-aromatic compounds. *Concept of Chirality:* Recognition of symmetry elements and chiral structures, stereoisomerism, determining absolute configuration. Optical activity and optical purity, Resolution, chiral chromatography, application of enzymes, chiral crown ethers and cyclodextrins. Conformation of carbocycles up to cyclodecane.

#### Unit II

Reactive intermediates: Structure stability and reactivity of intermediates, Generation and structure of carbocation, the concept of classical and non-classical carbocations, reactions involving carbocations, Carbanion, structure and reactivity, generation and reactions. Structure and reactivity of free radicals, carbenes and nitrenes as intermediates, their structure, generation and reactions. Aryne mechanism and ways of generation and their reactions. Introduction to heterynes and reactions.

#### Unit III

Reactions, mechanism and applications of the following name reactions: Bayer-Villiger oxidation, Dakin reaction, Baker-Venkataraman reaction, Reformatsky reaction, Robinson annulation, Cannizzaro reaction, Dieckmann reaction, Perkin Reaction, Stobbe condensation, Bischler-Napieralski reaction, Wittig rearrangement.

#### Books Recommended:

1. Advanced Organic Chemistry, Jerry March
2. Physical Organic Chemistry, Jack Hine
3. Organic Chemistry, Stanley H. Pine
4. Organic Reactions, Ed. Roger Adams and A. C. Cope.
5. The Modern Structural Theory of Organic Chemistry, L.N. Ferguson
6. Comprehensive Organic Chemistry -D. H. R. Barton Vols.1-6.
7. Organic Chemistry -R.T. Morrison and R. N. Boyd, 6<sup>th</sup> Edition
8. Guidebook to Mechanisms in Organic Chemistry, P. Sykes
9. Synthetic Approaches in Organic Chemistry, R. K. Bansal
10. Reaction Mechanisms in Organic Chemistry, S. M. Mukherjee and S. P. Singh
11. Organic Reaction mechanisms, V.K. Ahluwalia, R.K. Parashar, Narosa Publ. 2002
12. Vogel's Textbook of Practical Organic Chemistry, Revised by B. S. Furniss, A. J. Hannaford, P.W.G. Smith, A. R. Tatchel.
13. Stereochemistry of Carbon Compounds, E. L. Eliel
14. Stereochemistry of Organic Compounds, D. Nasipuri
15. Stereochemistry of Organic Compounds, P. S. Kalsi
16. Name Reactions - A Collection of Detailed reaction Mechanisms, Li Jie Jack, Springer, NY.
17. Name Reactions in Organic Synthesis, A. R. Parikh, H. Parikh and K. Parikh, Foundation Books, New Delhi



## Course CHE2203

### Physical Chemistry-2[3credits]

#### Unit I

*Adsorption and catalysis:* Heat of adsorption, Langmuir and BET isotherms, estimation of surface area, kinetics and thermodynamics of chemisorption. Adsorption in liquid systems and surface films. General features of homogeneous and heterogeneous catalysis, catalytic activity and strength of chemisorption, sticking probability, kinetics of adsorption and desorption, promoters and poisons, catalyst support, methods of preparation of heterogeneous catalysts, catalyst characterization, Important industrial catalysts (three), phase transfer catalysis.

#### Unit II

*Electrochemistry:* Electrical double layer: Structure of electrical interface, parallel plate condenser model, Gouy-Chapmann diffused charge model, Stern model, limitations of these models. Thermodynamics and kinetics of electrochemical metal deposition and dissolution process (corrosion), mechanism, Local cell theory, corrosion current, Evan's diagram, Protection and prevention of corrosion.

#### Unit III

*Statistical thermodynamics:* Limitations of classical thermodynamics. Introduction to the terms like ensemble, population, equipartition of energy, degeneracy. Boltzmann's distribution law, Evaluation of  $\beta$ , partition function, Distinguishable and indistinguishable particles, molar partition function, Electronic, Translational, Rotational and Vibrational partition functions, Sackur-Tetrode equation, preliminary treatment of Onsager reciprocal relation.

#### Books Recommended:

1. Bockris, J. O'M. and Reddy, A. K. N. (1998) *Modern Electrochemistry*, Vol. 2 A & B, Second Edition, Plenum Press, New York.
2. Chakrabarty, D. K. (Reprint 2007), *Adsorption and Catalysis by Solids*, New Age International Publishers, New Delhi.
3. Bond, G. C. (1974), *Heterogeneous catalysis: Principles and applications* Clarendon Press, Oxford
4. Terry L. Hill, (1987) *Introduction of Statistical Thermodynamics*, First Edition, Dover Publications, New York.
5. M. C. Gupta, (1990) *Statistical Thermodynamics*, Second edition, New Age International Publications, New Delhi
6. T. Engel and P. Reid, (2007) *Thermodynamics: Statistical Thermodynamics and Kinetics*, First Edition, Pearson Education, Noida

.....

## Course CHE2204



## Analytical Techniques-II [3credits]

### Unit I Statistics for chemists

Sources of variation in data, confidence limits of mean, significance test, Comparison of means, paired test, F test for variance, outliers.

*Errors in instrumental analysis:* Calibration curves, line of regression, errors in slope and intercept.

### Unit II Analytical Techniques

*Electrogravimetry:* Principle, Electrolysis at controlled potentials and electrolytic separations. Controlled potential coulometry, working of coulometer, coulometric titrations and applications.

Solvent extraction.

### Unit III Good Laboratory Practices and Environmental Chemistry

GLP Principles, Documentation of laboratory work, Preparation of Standard Operating Procedures (SOPs), Validation of methods, Reporting and documentation of results, Quality Control and Quality Assurance, Types of Quality Standards for laboratories, Total Quality Management, Audits

*Environmental Chemistry:*

Chemical Speciation and toxicity of particulate, gaseous and soluble pollutants, remedial measures.

Methods of control of industrial air pollution.

### Books Recommended :

1. Statistics of analytical Chemistry: J. C. Miller & J. N. Miller,
2. Statistical Analysis method for chemists - A software based approach. W.P. Gardiner, The Royal Society of Chemistry, 1997.
3. Modern Analytical Chemistry, D. Harvey , McGraw Hill, 2000
4. Principles of Instrumental Analysis : Douglas Skoog, Pearson
5. Introduction to Instrumental Analysis: Robert Brown
6. Instrumental Method of Analysis : H. H. Willard, L. L. Merritt & J.A. Dean
7. Instrumental Methods of Chemical Analysis, B.K. Sharma, Goel Pub's House)
8. Introduction to Thermogravimetric Analysis, C.J. Keattch and D. Dollimore.
9. Working with Ion selective Electrodes, O.K. Camman.
10. A textbook of Environmental Chemistry : O.D. Tyagi and M. Mehra , Anmol Pub.
11. Perspectives of Environmental Chemistry : Mc Cald
12. Environmental Inorganic Chemistry : Irgoli and Martell

.....

## Course CHE2205 Spectroscopy-II [4 credits]

**Unit I**

**Molecular Spectroscopy:** Interaction of electromagnetic radiation with matter and photophysical processes; Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. **Microwave spectroscopy:** Basic concept, rotation spectra of simple inorganic compounds, Classification of molecules, rigid rotor model, effect of isotopic substitution on transition frequencies & intensities non rigid rotor, Stark effect nuclear and electron spin interaction and effect of external field. Applications of Micro wave Spectroscopy.

**Infrared Spectroscopy:** Linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. Basic Instrumentation, Selection rules, normal modes of vibration, group frequencies, overtones, Fermi resonance, hot bands, factors affecting the band positions and intensities. FTIR. and NIR; applications.

**Unit II**

**Raman spectroscopy:** Rayleigh scattering, Raman Scattering. Polarizability, Polarization of Raman lines, Rule of mutual exclusion, Instrumentation and applications

**Electronic Spectroscopy:** Electronic states of diatomic molecules, Molecular term symbols, selection rules for diatomic molecules, Franck-Condon principle and intensities of electronic spectra. Electronic spectra of polyatomic molecules, Absorptions due to ethylenic and carbonyl chromophore, solvent effects on electronic spectra.

**Fluorescence Spectroscopy:** Fluorescence, and phosphorescence, fluorescence quenching concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photoexcited donor and acceptor systems (FRET). Stern-Volmer relation

**Unit III**

**Spectrometric Methods of Analysis:** Quantitative analysis using IR spectroscopy Quantitative analysis using UV-Visible spectroscopy: Relationship of  $\lambda_{\max}$  &  $\epsilon_{\max}$  to structure. Instrumentation Qualitative and Quantitative analysis: Determination of dissociation constant, Keto - enol tautomerism and stoichiometry, Spectrophotometric titrations. Derivative spectrometry, expanded scale spectrometry and reflectance spectrometry.

**Mass Spectrometric Technique:** Introduction to Mass Spectrometry - history and basics, magnetic sector instruments, Ion cyclotron and time-of-flight instruments, Quadrupoles and tandem MS instruments, ion traps, Sample inlet systems

**Unit IV**

**Mass Ionization techniques:** electron impact, chemical ionization, field desorption (FAB),\_electrospray, Interpretation of spectra.

**Structural elucidation of simple molecules using spectral data:** Molecular Formulae Index (D.B.E), Molecular ion peak, base peak, metastable ions, Nitrogen rule, effect of isotopes, Rules for fragmentation, McLafferty rearrangement, retro Diels-Alder fragmentation, Fragmentation of hydrocarbons, alcohols, Phenols, Halides, aldehydes, Ketones, amines, nitriles, carboxylic acids, esters, Problems based on analysis of mass spectra of various organic compounds Prediction of molecular formulae based on relative abundance.

1. Physical Methods in Chemistry : R.S. Drago, Saunders College
2. Modern Spectroscopy
3. Applied Electron Spectroscopy for Chemical Analysis : H. Windawi and F.L.Ho. , Wiley Interscience
4. NMR, NQR, EPR & Mossbauer Spectroscopy in Inorganic Chemistry : R.V. Parish, Ellis Harwood.
5. Introduction to Molecular Spectroscopy : G.M. Barrow, McGraw Hill

6. Basic Principles of Spectroscopy : R. Chang. McGraw Hill.
  7. Theory & Application of UV Spectroscopy : H.H. Jaffe and M. Orchin, IBH - Oxford.
  8. Investigations of Molecular Structure B.C. Gilbert ELBS:
  9. Nuclear Magnetic Resonance : P. J. Hoe , Oxford Science Publication.
  10. Fundamentals of Molecular Spectroscopy : C N Banwell. Tata McGraw.
  11. Molecular Structure and Spectroscopy - G. Aruldas, Prentice Hall of India
  12. Spectrometric Identification of Organic Compounds, R.M.Silverstein, F.X.Webster and D.Kimble, Wiley, New York
- .....

## Practical Courses

The following Experiments will be performed by the students during 1<sup>st</sup> and 2<sup>nd</sup> semesters as practical courses, CHE2106, CHE2107, CHE2108, CHE2109 (Semester1, 8 credits) and CHE2206, CHE2207, CHE2208, CHE2209 (semester2, 8 credits):

1. Qualitative analysis of mixtures containing at least six radicals including ions of two rare elements:
  - (a) Cations of : Ag, Pb, Hg, Cu, Cd, Sn, Bi, As, Sb, Fe, Al, Cr, Co, Ni, Mn, Zn, Ca, Sr, Ba, Mg, Na and K.  $\text{NH}_4^+$  .
  - (b) Cations of rare elements : W, Tl, Mo, Ce, Ti, Th, Zr, U, V, Be and Li.
  - (c) Anions :  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{NO}_2^-$ ,  $\text{NO}_3^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_3^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{S}_2\text{O}_3^{2-}$ ,  $\text{CrO}_4^{2-}$ ,  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{CO}_3^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{AsO}_3^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CH}_3\text{COO}^-$ ,  $\text{C}_2\text{O}_4^{2-}$  and  $\text{SiO}_4^{4-}$ .
2. Quantitative analysis of binary and ternary mixtures including analysis of rare elements.
 

Cations of : Ag, Cu, Cd, Fe, Co, Ni, Al, Mg, Ca, Ba and K .

Ions of rare Elements : W, U, Zr, Th, Ce and Mo .

Anions :  $\text{Cl}^-$ ,  $\text{NO}_2^-$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{SO}_4^{2-}$  and  $\text{S}_2\text{O}_3^{2-}$ .

Note: (1) Ions in bold will be estimated by gravimetric methods .

(2) Ions with underline will be estimated by volumetric methods.
3. Synthesis , analysis , and magnetic measurements of binary complexes ( at least five) of transition metal ions with monodentate and bidentate ligands like ammonia , thiocyanate, tertiary amines , ethylene diamine , acetylacetone .
4. Analysis of alloys : (any two)
 

Bronze , nickel based alloy , solder metal , white metal , duralumin.
5. Separation and identification of components of organic compounds(at least six).
6. Estimation of amino, methoxy and hydroxy groups, estimation of mixtures, acid and ester, acid and amide, estimation of starch content in turmeric powder, total reducing sugar content in honey.
7. Two stage organic preparations (at least seven).

8. Conductometry:

1. Strong base vs weak acid (Titration)
2. Precipitation titration  $\text{AgNO}_3$  vs  $\text{KCl}$ ;  $\text{AgNO}_3$  vs  $\text{KCl} + \text{KI}$
3. Dissociation constant by dilution method
4. Solubility product
5. Isoelectric point
6. Hydrolysis constant of a given salt
7. CMC of surfactant by conductometric method.

9. Potentiometry :

1. Mixture of weak acid and strong acid
2. Precipitation titration
3. Redox potential
4.  $\text{pK}_1$  and  $\text{pK}_2$  by titration method
5. Dissociation constants by dilution method
6. Solubility product

10. pH Metry :

1. Mixture titration
2.  $\text{pK}_1$  and  $\text{pK}_2$

11. Visible Spectrometry :

1. Determination  $\lambda_{\text{max}}$  and concentration of  $\text{KMnO}_4$  solution
2. Analysis of mixture of  $\text{CoSO}_4$  and  $\text{NiSO}_4$
3. pH - indicator - Dissociation constant

12. Kinetics :

1. Energy of activation for hydrolysis of methyl acetate
2. Relative strength of the acids by Polarimetry.

13. Molecular weight of polymer by Viscometry

14. CMC by Surface Tension measurement

15. Determination of salt concentration by ion exchange method.

16. Phase diagram : Phenol - Water System.

17. Dilatometry : Decomposition of diacetone alcohol.

18. Determination of  $\text{Cu(II)}$  by Spectrophotometric titration.

19. Estimation of detergents by Coulometry.

20. Assay of folic acid tablet (Folic acid)

21. Estimation of  $\text{Na}^+$  &  $\text{K}^+$  individually & in binary mixture by flame photometry.

22. Estimation of quinine by fluorimetry

23. Determination of purity of vanillin by conductometry

24. Assay of aspirin tablet by potentiometry

25. Paper chromatographic separation of metal ions ( $\text{Pb}^{2+}$ ,  $\text{Ag}^+$  and  $\text{Hg}^{2+}$ )

26. TLC separation of sugars and amino acids

27. Column chromatographic separation and estimation of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$

28. Determination of purity of ascorbic acid.

29. Determination of COD of effluent sample.

30. Analysis of oils

31. Quantitative determination of methanol and ethanol by GC.