# Syllabus M.Sc. (Chemistry) (MSCCHEM)

# **Semester 1**

# MCH-011: INORGANIC CHEMISTRY-I

(04 Credits, 60 Lectures)

**General Characteristics of Main Group Elements and Transition Elements** :Periodic Trends of Main Group Elements and Transition Elements; Electronic Configuration (Along with IUPAC Periodic Table), Periodic Trends in Properties, Atomic Radii, Atomic Volume and Density, Melting and Boiling Points, Ionisation Energy, Electronegativity, Electrode Potential, Oxidation States; Stability of various Oxidation States for Mn, Fe and Cu; Latimer Diagrams

**The Structure of Molecules(4 lectures):** VSEPR (Along with Point Groups); Walsh Diagram (Triatomic and Penta-atomic Molecules), $d\pi$ -p $\pi$  Bond; Bent Rule and Energetics of Hybridization; Geometric and Optical Isomers

**Phosphorus-nitrogen and Sulfur-nitrogen Compounds:** Phosphorus-nitrogen Compounds; Synthesis, Structure, Bonding and Uses of Cyclo and Linear Phosphonitrilic Compounds; Sulphur-Nitrogen Compounds; Ring and Chain Compounds  $S_2N_2$ ,  $S_4N_4$ . (SN)<sub>x</sub> etc.

**Organometallic Compounds:** Classification and Nomenclature of Organometallic Compounds; Organometallic Compounds of Alkali and Alkaline Earth Metals; Synthesis, Structure and Bonding, Properties and Uses; Organometallic Compounds of Transition Metals; Alkyls and Aryls Types, Routes of Synthesis, Stability and Decomposition Pathways, Organocopper Compounds and Its Applications

**Metal Carbonyls:**Metal Carbonyl; 18-electron Rule, Counting Electrons in Complexes, Structure and Bonding; Important Reactions of Metal Carbonyls; Vibrational Spectra of Metal Carbonyls; Bonding and Structural Elucidation of Carbonyls

**Metal pi-Complexes:**Transition Metal Nitrosyl Complexes; Transition Metal Dinitrogen and Dioxygen Complexes; Tertiary Phosphine as Ligand; Alkene, Alkyne, AllylDiene and Cyclopentadienyl Complexes; Arenes and Other Alicyclic Ligands

**Metal Clusters:**Higher Boranes, Wade's Rules; Carboranes, Metalloboranes and Metallocarboranes; Compounds with Metal-metal Multiple Bonds

**Crystal Field Theory :** Crystal Field Theory; Octahedral Complexes; Splitting of Orbitals ay An Octahedral Field, Spectrochemical Series, Crystal Field Stabilization Energy, Weak and Strong Field Complexes, Pairing Energies, Low Spin and High Spin Complexes; Jahn Teller Effect ; Tetrahedral and Square Planar Complexes

**Applications and Limitation of Crystal Field Theory:** Applications of Crystal Field Theory; Lattice Energies, Ionic Radii, Thermodynamic and Related Aspects of Crystal Fields, Heats of Ligation, Site Preference Energies; Limitation of Crystal Field Theory; Molecular Orbital Theory, Nephelauxetic Effect; Pi-Bonding and Molecular Orbital Theory

**Basics of Magnetochemistry :** Definitions of Magnetic Properties; Types of Magnetic Bodies, Paramagnetism: Orbital & Spin Contribution; Magnetic properties; Lanthanoids, First Transition Metal Ions, Actinoids; Methods for Magnetic Susceptibility Measurements; Derivation of Van Vleck Equation *d*-metal Complexes: Magnetism: Ferromagnetism and Antiferromagnetism; Mechanism of Anti-Ferromagnetic Interaction; Spin Cross Over and Anomalous Magnetic Moments; Applications of Magnetic Measurement for Structural Elucidation

**Electronic Spectra of Transition Metal Complexes:** Spectroscopic Terms; R-S Coupling of  $d^{\circ}$  System, Racah Parameters, Correlation of Spectroscopic Terms; Orgel and Tanabe-Sugano Diagrams for Transition Metal Complexes ( $d^{\circ}-d^{\circ}$  states)

*d-d* transition and Charge Transfer Spectra: Selection Rules and *d-d* transition in Metal Complexes; Charge Transfer Spectra; LMCT Transitions, MLCT Transitions, The Nephelauxetic Series; Spectroscopic Method of Assignment of Absolute Configuration in Optically Active Metal Chelates and their Stereochemical Information; Inter-Valence

# **Further Reading:**

- 1. Advanced Inorganic Chemistry, F.A. Cotton and G.Wilkinson, John Wiley.
- 2. Inorganic Chemistry (4th ed.), J.E Huheey, Keiter, Keiter and Medhi, PearsonEducation, 2006.
- 3. Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Elements of Magnetochemistry (2<sup>nd</sup> Edition), R. L. Dutta & Syamal, EWP, New Delhi.
- 6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillard and J.A. McCleverty, Pergamon.

# MCH-012: STEREOCHEMISTRY AND REACTIVE INTERMEDIATES (4 credits, 60 Lectures)

(30 Lectures)

# Section A: Stereochemistry of Organic Compounds

**Molecular Symmetry and Chirality (3lectures):** Classification of Stereoisomers; Optical Isomers; Symmetry Operations and Symmetry Elements, Point Group Classification; Symmetry and Molecular Properties; Rotation of Polarised Light, Symmetry Number; Molecules with One Chiral Centre; Chirality and Symmetry

**Stereoisomerism of Molecules with More than One Chiral Centres(4lectures):** Molecules with Two Chiral Centres; Racemic Modifications, Formation(by mixing, synthesis, racemisation etc.), Properties, Different Methods of Resolution, Criteria of Optical Purity; Molecules with Three or More Chiral Centres; Axial and Planar Chirality and Helicity (P and M); Cyclostereoisomerism

**Conformations of Six-membered Rings:**Basic Aspects of Conformations; Stereochemistry of Cycloalkanes; Conformations and Stability of Cyclohexanes; Monosubstituted Cyclohexanes, Disubstituted Cyclohexanes, Trisubstituted Cyclohexanes; Conformations and Stability of Cyclohexanones and Halocyclohexanones; Cyclohexanones, Halocyclohexanones; Conformations and Stability of Decalins, Decalols, Decalones

**Stereochemistry of Complex Systems:** Stereochemistry of Allenes and Spiranes; Stereochemistry of Alkylidines, Stereochemistry of Ethanal, Propanal and Ethyl Methyl Ketone; Stereochemistry of Adamantanes; Stereochemistry of Catenanes; Stereochemistry of Biphenyls, Atropisomerism; Stereochemistry of Bridged Biphenyls; Stereochemistry of Ansa Compounds and Cyclophanes

**Configuration and its Correlation:** Representation of Configuration: *D, L, R, S* and *E, Z*-nomenclature; Determination of Configuration-Different Methods; Chemical Correlation, Quasiracemates

**Topicity and Prostereoisomerism:**Topicity of Ligands and Faces and their Nomenclature; Stereogenicity; Chirogenicity; Pseudoasymmetry; Stereogenic and Prochiral Centres

**Asymmetric Induction :**Cram's, Prelog's and Felkin-Ahn Model; Dynamic Stereochemistry (Acyclic and Cyclic); Qualitative Correlation between Conformation and Reactivity; Curtin-Hammett Principle

**Molecular Dissymmetry and Chiroptical Properties:**Linear and Circularly Polarised Lights; Circular Birefringence and Circular Dichroism; ORD and CD Curves; Cotton Effect; The Axial Haloketone Rule; Octant Diagrams; Helicity; Lowe's Rule; Application of ORD and CD to Structural and Stereochemical Problems

# Section B: Reactive Intermediates in Organic Chemistry

(30Lectures)

**Organic Reaction Mechanisms:**Basic Aspects of Organic Reaction Mechanisms, HSAB principle and its Applications; Methods of Determination of Organic Reaction Mechanisms; Linear Free Energy Relationships and their Applications (Hammett Equation and Modifications)

**Carbocations-I: Structural Aspects:**Structure and Stability of Carbocations; Classical and Non-Classical Carbocations; Neighbouring Group Participation; Ion-pairs

**Carbocations-II: Rearrangement Reactions:**Recapitulation of General Reactions; Molecular Rearrangements in; Acyclic Systems, Monocyclic Systems, Bicyclic Systems; Stability and Reactivity of Bridge-Head Carbocations

**Carbanions:**Generation of Carbanions; Structure and Stability of Carbanions; Ambident ions and their General Reactions; Rearrangements of Carbanions

**Free Radicals**:Generation of Free Radicals; Structure of Free Radicals; Stability and Reactions; Cage Effects; Radical-cations and Radical-anions; S<sub>R</sub>N1 Mechanisms

**Carbenes:**Formation and Structure of Carbenes; Reactions Involving Carbenes and Carbenoids, Electrophilic and Nucleophilic Reactions; Carbenoids

Nitrenes(3 lectures): Generation of Nitrenes; Structure and Reactions of Nitrenes

**Arynes:**Generation and Reactivity; Nucleophilic Aromatic Substitution Reactions; S<sub>N</sub>Ar Mechanism, Regioselectivity; Ipso Effect

# **Further Readings**

- 1. Carey, F.A. &Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2007) /LATEST EDITION.
- 2. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers (2003).
- 3. Finar, I. L. Organic Chemistry Vol. 1, Longman (1998).
- 4. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981)..
- 5. March, J. Advanced Organic Chemistry John Wiley & Sons (2004).
- 6. Kalsi, P. S. Stereochemistry: Conformation and Mechanism, 7th Edition New Age International, Delhi (2008).
- 7. Jonathan Clayden , Nick Greeves , Stuart Warren Organic Chemistry 2nd Edition

# MCH-013: GENERAL PHYSICAL CHEMISTRY (4 Credits, 60 Lectures)

**Gibbs and Helmholtz's Functions(3lectures):** Laws of Thermodynamics; Gibb's Function and Equilibrium Criterion; Temperature and Pressure Dependence of Gibb's Energy; Helmholtz Function and Equilibrium Criterion

**Systems of Variable Composition(3lectures):**Partial Molar Quantities and Their Significance, Experimental Determination Partial Molar Volume; Chemical Potential, Significance of Chemical Potential; Mixture of Gases, Fugacity and Its Significance; Gibbs-Duhem Equation

**Introduction to Statistical Thermodynamics:** Basic Probability Theory; Permutations and Configurations, Stirling Approximation; Probability Distribution Functions; Characteristics of Probability Distribution Functions; Boltzmann's Distribution; Microstates and Configurations, Physical Significance; Canonical Ensemble; Molecular Partition Functions; Translational PartitionFunctions, Rotation PartitionFunctions, Vibration PartitionFunctions, Electronic PartitionFunctions; Third Law of Thermodynamics

**Fundamentals of Solid State:**Solid State and Its Characteristics; Crystal Lattice, Designation of Lattice Planes; X-Ray Diffraction, Indexing Crystal Planes; Electronic Structure of Solids; Magnetic Properties of Solids, Curie and Curie-Weiss Laws, Calculation of Magnetic Moments

**Crystal Symmetry:**Molecular Symmetry, Symmetry Elements versus Symmetry Operations; Crystal Symmetry; Screw Axis, Glide Plane; Stereographic Projections

**Collision and Transition State Theories:**Collision theory and Its Limitations, Limitations of Collision Theory; Transition State Theory; Thermodynamic Approach, Statistical Approach,

**Theories of Unimolecular Reactions(4lectures):** Unimolecular Reactions and Their Characteristics; Lindemann's Mechanism; Experimental Verification, Limitations of Lindemann's Mechanism; Hinshelwood's Theory, Limitations of Hinshelwood's Theory; RRKM Treatment

**Kinetics of Reactions in Solution(3lectures):** Role of Solvents in Reactions in Solution; Theory of Reaction Rate in Solution; Salt Effects; Primary Salt Effects, Secondary Salt Effects

**Kinetics of Fast Reactions:**Fast Reactions and Their Importance; Flow Techniques; Continuous Flow Technique,Accelerated Flow Method, Stopped Flow Method, Limitations of Flow Techniques; Relaxation Methods; Shock Tubes, Flash Photolysis,Laser Photolysis; Spectroscopic Techniques

**Kinetics of Enzyme Reactions:**Enzymatic Reactions And Their Characteristics; The Michaelis–Menten Mechanism, Turnover Number and Michaelis Constant, Lineweaver–Burk Plot; Mechanisms of Enzyme Inhibition; Competitive Inhibition, Non-Competitive Inhibition

**Catalysis:** Adsorption Phenomenon, Langmuir Adsorption Isotherm; Gibbs Adsorption Isotherm; Multilayer Adsorption, Bet Equation and Its ApplicationHeterogenous Catalysis

**Debye Huckel Theory-I:**Ionic Cloud, Poisson's Equation;Non-Idealityof Electrolytic Solutions; Activity and Mean Activity Coefficient, Measurement of Activity Coefficients; Debye Huckel Theory; Postulates of Debye Huckel Theory, Mathematical Treatment;

**Debye Huckel Theory-II:** Ionic Cloud and Electrostatic Potential; Charge Distribution around Central Ion, Chemical Potential Changes Due To Ion-Ion Interactions; Success And Limitations of Debye Huckel Theory, Modification in Huckel Law; Mean Ionic Activity Coefficients, Determination of Mean Ionic Activity Coefficients

**Diffusion and Viscosity:** Transport Phenomenon; Kinetic Theory of Gases; Distribution of Molecular Velocities, Mean Free Path; Diffusion Across Concentration Gradient; Fick's First Law of Diffusion, Relationship between Diffusion Coefficient and Mean Free Path; Viscosity and Coefficient of Viscosity; Osmosis; Diffusion versus Osmosis, Reverse Osmosis, Forward Osmosis

**Thermal and Electrical Conduction:** Thermal Conduction, Coefficient of Thermal Conductivity and Mean Free Path; Electrical Conduction; Drift Velocity, Relationship between Ionic Mobility and Conductance

### **Further Readings**

- 1. Klotz Irving M. and Rosenberg Robert M. Chemical Thermodynamics: Basic Concepts and Methods; Wiley-Interscience; 7th edition (2008)
- 2. J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry 1 (Ionics), Springer (2006).
- 3. Laidler, K. J. Chemical Kinetics 3rd Ed., Benjamin Cummings (1997).
- 4. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)
- 5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
- 6. West, A.R. Solid State Chemistry & its Applications, John Wiley & Sons (1987).
- 7. West, A.R. Basic Solid State Chemistry, 2nd Edition, John Wiley & Sons (2000).
- 8. Smart, L.E. & Moore, E.A. Solid State Chemistry An Introduction, 3rd Edition, CRC Press (2005).
- 9. Brett, C. M. A. & Brett, A. M. O. Electrochemistry Oxford University Press (1993).
- 10. McQuarrie, D. A. Statistical Mechanics Viva Books Pvt. Ltd.: New Delhi (2003).
- 11. Nash, L. K. Elements of Statistical Thermodynamics 2nd Ed., Addison Wesley (1974).
- 12. McQuarrie, A. Donald and John D Simon. Molecular thermodynamics.California: University Science Books 1999.
- 13. S. Glasstone, Thermodynamics for Chemists, New Delhi: MauricePress, 2008.

# MCHL-011: CHEMISTRY LAB-I

(2 Credits, 60 Lectures)

### Semimicro Qualitative and Quantitative Analysis

- 1. Detection of less common metal ions: Ce, Ti, Mo, W, Zr, Th, V, U, (two metal ions in cationic/anionic forms: minimum two mixtures).
- 2. Separation and determination of two metal ions (Ca, Mg, Cu, Ni, Zn, Cu, Pb) involving volumetric titrations (redox & complexometry) and gravimetry (minimum four experiments).

### **Further Readings:**

- 1. Vogel's Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J. Mendham, ELBS.
- 2. Introduction to Semimicro Qualitative Analysis by J.J. Lagowski and C.H. Sorum, Prentice Hall, Englewood Cliffs, N.J.
- 3. Vogel's Textbook of Qualitative Analysis, revised by G. Svehla, Orient Longman.

# MCHL-012: CHEMISTRY LAB- II

- A) Identification of components in a two-component mixture and preparation of their derivatives.
   Determination of b.p. / m.p. for components and m.p. for the derivatives. (3+3 mixtures) 3 days (6 Session)
- B) Any **Six preparations** from the following:
- 1. Preparation of o-benzoyl benzoic acid (Fridel Crafts Reaction)
- 2. p-Nitrobenzoic acid from p-nitrotoluene (Oxidation)
- 3. Anthroquinone from anthracene (Oxidation)

5

3 days (6 Sessions)

(2 Credits, 60 Lectures)

- 4. Glucose pentaacetate from Glucose (Acetylation)
- 5. m-Nitroaniline from m-dinitrobenzene (Reduction)
- 6. Benzophenoneoxime from benzophenone (Addition reaction)
- 7. p-Chlorotoluene from p-toluidine (Sandmeyers' Reaction)
- 8. 2,3 Dimethylindole from phenyl hydrazine and 2 butanone (Fisher Indole Synthesis)
- 9. 1,2,3,4 Tetrahydrocarbazole from cyclohexanone (Fisher Indole Synthesis)
- 10. Methyl orange from sulphanilic acid (Diazo Reaction)

### **Further Readings:**

- 1. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).
- 2. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).
- Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

# MCHL-013: CHEMISTRY LAB-III

(2 Credits, 60 Lectures)

# Note: Perform any ten of the following experiments

Expt. No.	Title of the Experiment
1	To determine the partial molar volumes of sodium chloride solutions by measuring function of concentration, using a pycnometer.
2	Determine the mean activity coefficient ( $\gamma$ ) of 0.01 M hydrochloric acid solution.
3	Determination of the specific rate constant for the acid catalysed hydrolysis of methyl acetate using hydrochloric acid at two temperatures by Initial Rate Method and calculate the thermodynamic parameters
4	To determine the molecular weight of a given macromolecule (PVP) by the viscosity method.
5	To verify Gibb's adsorption isotherm and determine the surface area of charcoal.
6	Set up saturated calomel electrode and measure its potential using the quinhydrone electrode as reference electrode.
7	To set up the Zn/ZnSO <sub>4</sub> (0.1 M)electrode, measure its potential and obtain the value for its standard electrode potential
8	To determine the concentration of sodium carbonate in a commercial sample of soda ash by conductometric titration with hydrochloric acid.
9	To determine the strength of a moderately strong acid (salicylic/ mandelic acid) by conductometric titration using(a) salt-line method or (b) double alkali method.
10	To study the effect of dielectric constant ( $\epsilon$ ) on the nature of the conductometric titration between maleic acid and sodium methoxide using different combinations of methanol and hexane as solvents.
11	To study the stepwise neutralisation of oxalic acid or citric acid by

conductometric titration and explain the variation in the plots.

- 12 To determine the dissociation constant of acetic acid potentiometrically.
- 13 To determine molar conductivity of a strong electrolyte at different concentrations and verify Debye-Hückel-Onsager equation.

### **Further Readings:**

- 1. Experiments in Physical Chemistry, Carl W. Garland, Joseph W. Nibler, David P. Shoemaker, Mcgraw-hill
- 2. Experimental Physical Chemistry, Mathews, G. Peter, Oxford Clarendon Press (1985).
- 3. Levitt, Findlay's practical physical chemistry. Longman's London: 1966.
- 4. A.M. James and D.E. Pritchard. Practical physical chemistry, Longman Group Ltd: 1968.
- 5. V.D. Athawale and Parul mathur. Experimental physical Chemistry. New Age International: New Delhi, 2001.

# MCH-014: MATHEMATICS FOR CHEMISTS (2 Credits, 30 Lectures)

**Differential Calculus:** Limits and Continuity; Differentiation; Rules of Differentiation, Chain Rule, Differentiation by Substitution; Application of Differentiation; Maxima and Minima, Bohr's Radius, Most Probable Velocity; Exact and Inexact Differentials, Applications; Functions of Two or More Variables; Partial Differentiation, Transformation of Coordinates

**Integral Calculus:**Methods of Integration; Standard Integrals, Method of Substitution, Transformation of Trigonometric Integrands, Integration by Parts, Integration of Algebraic Fractions; Definite Integrals; Properties of Definite Integrals, Applications of Definite Integrals

**Elementary Differential Equations:**Ordinary Differential Equations; Classification of Differential Equations, Solution of Ordinary Differential Equations; First Order First Degree Equations; First Order Second Degree Equations, Applications; Second Order Differential Equations Applications; Partial Differential Equations, Applications

**Experimental Errors, Probability, and Statistics:** Probability and Probability Theorems; Systematic and Random Errors, Distribution of Errors; The Method of Least Squares and Curve Fitting; Principle of Least Squares, Fitting of Data to a Linear Function, Fitting of Data to Other Functions; Significance Tests; Significance Levels, The u-test, Student's t-test, □<sup>1</sup>test, Applications of Significance Tests

**Introduction to Vectors (4 lectures):** Vectors and Scalers, Electronic Configuration (Along with IUPAC Periodic Table); Dot and Cross Product of Vectors, Latimer Diagrams; Gradient, Divergence and Curl

**Matrix Algebra-I** :Addition and multiplication of Matrices; Inverse, Adjoint and Transpose of Matrices; Special matrices and Their Properties; Symmetric and Skew-symmetric Matrices, Hermitian and Skew-Hermitian Matrices, Unit Diagonal and Unitary Matrices; Determinant of a Matrix

**Matrix Algebra-II**: Solution of simultaneous equations; Homogeneous Linear Equations; Nonhomogeneous Linear Equations; Linear Dependence and Independence; Matrix Eigenvalues and Eigenvectors

- 1. Mortimer, R. G. Mathematics for Physical Chemistry 2<sup>nd</sup> Ed. Elsevier (2005).
- 2. Kreyszig, E., Advanced Engineering Mathematics, John Wiley & Sons, Inc. (2006)
- 3. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
- 4. Mathematics for Chemistry, Doggett and Sutliffe, Longman.

- 5. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
- 6. Chemical Mathematics, D.M. Hirst, Longman.
- 7. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
- 8. Basic Mathematics for Chemists, TebbJtt, Wiley.

# MCH-015: BIOLOGY FOR CHEMISTS

(2 Credits, 30 Lectures)

**Cell and Cell Organelles :** Cell Structure, Structure of Prokaryotic and Eukaryotic Cells; Cell Organelles, Intracellular Organelles and Their Functions; Plant versus Animal Cells, Biological functions of micelles, bilayers, liposomes; Origin of Life ; Unique Properties of Carbon, Chemical Evolution; Biological Membranes; Fluid Mosaic Model, Transport Across Membranes

**Molecules of Life-I:**Introduction to Molecules of Life, Role of Water in Living Systems; Important Derivatives of Monosaccharides; Glycosides and Amino Sugars, Disaccharides and Polysaccharides, Glycosaminoglycans, Glycoproteins and Glycolipids; Glycoproteins and Glycolipids

**Molecules of Life-II:**Structure and Function of Lipids; Triacyclglycerols, Glycerophospholipids, Sphingolipids, Bile Acids, Prostaglandins; Lipoproteins; Composition and Function, Role in Atherosclerosis; Lipid Aggregates, Micelles, bilayers, liposomes; Proteins; Biological Functions and Their Structural Basis, Enzymes: Biological Function and Diagnostic Role

**Metabolism-I**: Overview of Metabolic Process; Catabolism and Anabolism, Intermediary Nature; Introduction to Bioenergetics; ATP- The Biological Energy Currency, Biochemical Standard State, Coupling Reactions, Universal Electron Carriers; Metabolism of Carbohydrates

Metabolism-II : Metabolism of Proteins; Metabolism of Fats; Metabolism of Nucleic Acids

**Homeostasis :**Need for Homeostasis; Regulation of Blood Glucose; Maintaining Water Balance; Acid-Base Balance; Thermoregulation

**Immune System :**Introduction to Immunity; Origin and Concept, Levels of Immunity, Levels of Defence, Types of Immunity; Cellular and Humoral Immune Response; Characteristics of Immune System; Immunoglobulins, Types and Structures; Theories of Immune Response; HLA Typing

**Genetics and Molecular Biology :** Introduction to Genetics, The Chemical Basis for Heredity; Central Dogma; Expression And Processing Of Biological Information; Replication, Transcription, Translation, Regulation; Molecular Biology; Recombinant DNA Techniques, Genetically Modified Organisms, Stem Cell Research

- 1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
- 2. Biochemistry, I.Stryer, W.H.Freeman.
- 3. Biochemistry, J. David Rawn, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry, E. E.Conn and P. K. Stumpf, John Wiley.

# MCH-016: INORGANIC CHEMISTRY-II (04 Credits, 60 Lectures)

**Reaction Mechanisms in Substitution Reactions I:** Mechanisms of Substitution Reactions of Square Planar Complexes; Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects; Mechanisms of Substitution Reactions of Trigonal Bipyramidal Complexes; Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects

**Reaction Mechanisms in Substitution Reactions II:** Mechanisms of Substitution Reactions of Square Pyramidal Complexes; Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects; Mechanisms of Substitution Reactions of Octahedral Complexes; Potential Energy Diagrams, Transition States and Intermediates, Isotope Effects

**Ligand Substitution in Square Planar Complexes :** Berry's Pseudo Rotation Mechanism; Factors Affecting the Reactivity of Square Planar Complexes, Swain-Scott Equation

**Ligand Substitution in Octahedral and Tetrahedral Complexes :** Trans Effect and its Application to Synthesis of Complexes; Stereochemical Changes in Substitution Reactions of Octahedral and Tetrahedral Complexes

**Molecular Rearrangements-I:** Molecular Rearrangement Processes; Electron Transfer Reactions (Outer and Inner Sphere); HOMO and LUMO of Oxidant and Reductant, Chemical Activation

**Molecular Rearrangements-II:** Precursor Complex Formation and Rearrangement; Nature of Bridged Ligands; Fission of Successor Complexes, Two-Electron Transfers

**Methods of Synthesis of Coordination Compounds :**Synthesis of Coordination Compounds Using Electron Transfer Reactions; Mixed Valence Complexes and Internal Electron Transfer

**Energy Sources for Life(6 lectures):** Ferritin, Transferrin and Siderophores; Hemoglobin and Myoglobin, Perutz Mechanism Models of Oxygen Carriers

Photosynthesis and Nitrogen Fixation : Photosynthesis PSI and PSII Systems; Nitrogen Fixation

**Metalloenzymes:** Zinc Enzymes-Carboxypeptidase and Carbonic Anhydrase; Iron Enzymes-Catalase; Peroxidase and Cytochrome P-450; Metalloenzyme-II; Copper Enzymes-Superoxide Dismutase; Molybdenum Exotransferase Enzymes-Xanthine Oxidase, Coenzyme Vitamin B12

**Metal-Nucleic Acid Interactions:** Metal-Nucleic Acid Interactions; Metal Complex – Nucleic Acid Interaction Modes of Binding to DNA, DNA Cleavage

**Metals in Medicine (6 Lectures):** Metals in Medicine, Metal Deficiency and Disease; Toxic Effects of Metals; Metals Used for Diagnosis and Chemotherapy with Particular Reference the Anticancer Drugs

- 1. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, John Wiley.
- 2. Inorganic Chemistry, J.E. Huheey, Harper & Row.
- 3. Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
- 6. Inorganic Chemistry, G. Wilysberg, University Science Books.
- 7. Physical Methods in Inorganic Chemistry, R. S. Drago.

- 8. Inorganic chemistry by D. F. Shriver, P. W. Atkins and C. H. Langford
- 9. Structural Methods in Inorganic Chemistry by Ebsworth.
- 10. An Introduction to Inorganic Chemistry by Purcell and Kotz
- 11. Mechanisms of Inorganic Reactions by R G Pearson, Fred Basolo

# MCH-017: ORGANIC CHEMISTRY-II

(04 Credits, 60 Lectures)

# Section A: Heterocycles and Organic Synthesis

Introduction to Heterocyclic Compounds :Nomenclature; Spectral Characteristics; Reactivity and Aromaticity

**Three Membered Heterocycles:**Synthesis and Reactions of Aziridine, Oxiranes and Thiarines; Synthesis and Reactions of Azirines

**Four Membered Heterocycles :**Synthesis and Reactions of Azetidine; Synthesis and Reactions of Oxetanes; Synthesis and Reactions of Thietanes

**Five Membered Heterocycles with Two Heteroatoms in Rings:**Synthesis and Reactions of Pyrazole; Synthesis and Reactions of Imidazole; Synthesis and Reactions of Oxazole; Synthesis and Reactions of Thiazole; Synthesis and Reactions of Isothiazole and Benzofused analogs

**BenzofusedFive Membered Heterocycles with One Heteroatom:**Synthesis and Reactions of Indole; Synthesis and Reactions of Benzofuran; Synthesis and Reactions of Benzothiophene

**Bicyclic Heterocycles Containing One or More Heteroatoms(3lectures):** Synthesis and Reactions of Benzimidazole; Synthesis and Reactions of Benzotriazole; Synthesis and Reactions of Purine

**Benzofused Six Membered Rings with More than One Heteroatoms:**Synthesis and Reactions of Benzopyrans; Synthesis and Reactions of Quinolines and Isoquinolines; Synthesis and Reactions of Phenoxazines and Phenothiazines

**Seven and Large Membered Heterocycles:**Synthesis and Reactions of Azepines; Synthesis and Reactions of Oxepines; Synthesis and Reactions of Thiepines; Chemistry of Porphyrins

# SECTION B: SYNTHESIS OF ORGANIC COMPOUNDS

# (30 LECTURES)

(30Lectures)

**Philosophy of Organic Synthesis:**Disconnection Approach; One Group and Two Group Disconnections; Reversal of Polarity; Chemoselectivity; One Group C-C Disconnections; Two Group C-C Disconnections; 1,3-difunctional and 1,5-difunctional Compounds; Tandem Reactions, Domino Reactions and Multi-component Reactions

**Applications of Pd (0) and Pd (II) Complexes in Organic Synthesis :**Coupling Reactions; Stille, Suzuki and Sonogashira Couplings; Heck Reaction and Negishi Couplings

**Reductions:**Catalytic Hydrogenation: Stereochemistry and Mechanism; Metal-liquid Ammonia Reductions: Stereo-selection and Mechanism; Homogeneous Hydrogenations; Mechanisms and Applications Using Rh, Ru and Other Metal Complexes

**Reductions using Hydride Transfer Reagents :**Sodium Borohydride; Sodium Cyanoborohydride; Lithium Aluminium Hydride and Alkoxy Substituted LAH Reducing Agents; DIBAL; Applications of Hydroboration (Reductions, Oxidations and Cabonylations); Diborane Coupling Reaction; Diisoamylborane, Thexylborane and 9-BBN; Isopinocamphenyl and Diisopinocamphenylboranes

**Oxidations :**Use of Oxidizing Reagents with Applications and Mechanism; DDQ, SeO<sub>2</sub>, TI(NO<sub>3</sub>)<sub>3</sub>, Ceric Ammonium Nitrate; Sharpless Asymmetric Epoxidation; Asymmetric Hydroxylation and Aminohydroxylation

**Enolates:**Thermodynamic Versus Kinetic Enolates; Enolate Equivalents and Enamines; Applications in Carbon-Carbon Bond Formation and Related Reactions; Applications in Chiral Synthesis

**Umpolung Reactions :**Sulphur Compounds; Nitro Compounds; LithiatedEthers and Related Compounds

**Principles and Applications of Phase Transfer Catalysis :**Crown Ethers; Polymer-Supported Reagents in Organic Synthesis

**Asymmetric Synthesis :**Development of Methodologies for Asymmetric Synthesis; Regioselectivity; Stereoselectivity; Diastereoselectivity and Stereospecificity

### **Further Reading**

- 1. "Heterocyclic Chemistry" by J A Joule and K Mills
- 2. Name Reactions in Heterocyclic Chemistry" by Jie Jack Li.
- 3. "Advances in Heterocyclic Chemistry" by Alan R Katritzky
- 4. Advanced Organic Chemistry-Reactions, Mechanism and Structure, M. B. Smith and Jerry March, John Wiley 2001.
- 5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum Publishers
- 6. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 7. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.
- 8. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
- 9. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.

# MCH-018: QUANTUM CHEMISTRY AND GROUP THEORY (04 Credits, 60 Lectures)

**Fundamentals of Quantum Chemistry:**Inadequacy Of Classical Mechanics; Blackbody Radiation, Photoelectric Effect, Heat Capacities at Low Temperature, Line Spectra, Wave-Particle Duality and Uncertainty Principle; Postulates of Quantum Mechanics; Well Behaved Wave Functions, Quantum Mechanical Operators, Expectation Value

**Operators and Their Significance:**Operators and Their Representation; Linear and Hermitian Operators; Commutation of Operators and Their Significance; Time Dependent and Time Independent Schrodinger Equations; Eigenvalue Problem and Orthonormal Sets

**Particle in A Box:** Particle in One Dimensional Box; Formulating Schrödinger Wave Equation, Boundary Conditions and Solution of Schrödinger Equation, Energy Level Diagram, Wave Functions and Probability Densities; Particle In Three-Dimensional Box; Formulating Schrödinger Wave Equation, Boundary Conditions and Solution of Schrödinger Equation, Energy Level Diagram, Concept of Degeneracy, Wave Functions and Probability Densities; Application of Particle in One Dimensional Box

**Simple Harmonic Oscillator** :Linear Harmonic Oscillator: Classical Treatment; Linear harmonic Oscillator; Formulating Schrödinger Wave Equation and Boundary Conditions, Solution of Schrödinger Equation: Series Solution Method, Quantised Vibrational Energies, Wave Functions for Linear Harmonic Oscillator, Average Values Of Kinetic And Potential Energies; Virial Theorem

**Rigid Rotor:**Rotational Motion: Classical Treatment; Rigid Rotor; Formulating Schrodinger Wave Equation, Separation of Variables; Solving 
□ Equation; Solving □ Equation

**Hydrogen Atom-I(4 lectures):**Hydrogen Atom, Formulating Schrodinger Wave Equation; Solving Schrodinger Wave Equation; Separation of Variables, Results of Solutions of  $\Box \Box \Box$ , and R Equations; Quantum Numbers and Their Significance

**Hydrogen Atom-II:**Hydrogen Like Wave Functions; Radial Wave Functions, Angular Wave Functions (Spherical Harmonics), Radial Distribution Functions; Electron Spin and Spin Quantum Number

**Angular Momentum :**Classical Angular Momentum; Conservation of Angular Momentum, Representation of Angular Momentum; Angular Momentum In Quantum Mechanics; Orbital Angular Momentum, Spin Angular Momentum, Total Angular Momentum; Russel Saunders's Coupling

**Approximation Methods:**Variation Method and Its Applications; One Dimensional Box, Harmonic Oscillator, Hydrogen Atom; Perturbation Theorem

**Multi Electron Atoms:**Helium Atom, Formulation of Schrodinger Wave Equation; Approximating Energy; Ground State Energy of Helium Atom; First Order Perturbation, Variation Method ; Indistinguishability of Electron Spins, Pauli's Exclusion Principle; Multi Electron Atoms, Distribution of Electrons

**Molecular Symmetry and Groups:**Symmetry Operations and Elements, Molecular Symmetry Elements; Point Groups; Schoenflies System, Classification of Molecules Into Point Groups; Groups and Their Characteristics, Group Multiplication Tables

**Representations of Groups:** Matrix Representation And Its Characteristics; Basis for Representation, Similarity Transformations, Character of Representations; Irreducible Representation, Wavefunction as Basis for Representation; Great Orthogonality Theorem, Construction of Character Tables; Reduced Representation, Reduction of Representation; Symmetry Adapted Basis; Vanishing Integrals

**Valence Bond Theory:**Born-Oppenheimer's Approximation; Hydrogen Molecule, Coulomb's Integral, Exchange Integral, Overlap Integral; Polyatomic Molecules, Configuration Interaction

**Molecular Orbital Theory-I:**Born-Oppenheimer's Approximation; Hydrogen Molecule Ion; LCAO-MO Approach, Resonance and Overlap Integrals, Bonding and Antibonding Orbitals; Hydrogen Molecule

**Molecular Orbital Theory-II:**Homonuclear Diatomic Molecules, MO Configuration; Heteronuclear Diatomic Molecules; HF, LIF, CO; Polyatomic Molecules, Hybridisation

**Hückel Molecular Orbital Theory:**Hückel Molecular Orbital (HMO) Theory; Hückel Approximation, Applications of HMO; Extended Hückel Theory (EHT), Applications of EHT; Limitations of HMO and EHT

- 1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
- 2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt Ltd.: New Delhi (2003).
- 3. Pilar F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
- 4. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
- 5. Levine, I. L. Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
- 6. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
- 7. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
- 8. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley (2004)
- 9. F. A. Cotton, Chemical Applications of Group Theory, Wiley Eastern, 1990.
- 10. L. Robert Carter, Molecular Symmetry & Group Theory, John Wiley& Sons Inc Sea Pte Ltd, 2012.
- 11. K. Veera Reddy, Symmetry and Molecular Spectroscopy, New Age International Publishers, 2012.

# MCH-019: GREEN CHEMISTRY

(02 Credits, 30 Lectures)

**Green Chemistry:** The Need and Origin of Green Chemistry; Principles of Green Chemistry; Concept of atom Economy

**Tools of Green Chemistry:** Use of Alternatives; Feed Stocks/Starting Materials; Reagents; Solvents; Product/Target Molecules; Catalysis and Process Analytical Chemistry

**Evaluation of Chemical Products or Processes:** Effects on Human Health and Environment; Evaluation of Reaction Types; Methods to Design Safer Chemicals

Harmful Effects of Chemistry: Toxicity to Humans, Toxicity to Wildlife, Effects on Local Environment, Global Environmental Effects

**Planning a Green Synthesis:** Green synthesis of Ibuprofen; Design and Application of Surfactants for Carbon Dioxide for Precision Cleaning in Manufacturing and Service Industries

**Towards Safer Environment:** Microbes as Environmentally Benign Synthetic Catalysts; Safe Marine Antifoulants; Use of Molting Agents (To Replace More Toxic and Environmentally Harmful Insecticides)

**Using Safer Reagents:** Carbon Dioxide as Blowing Agent; Oxidant Activators to Replace Chlorine Based Delignification Process in Paper and Pulp Industry

**Greener Technologies:** Polyester Regeneration Technology; Biodegradable Polyaspartate Polymers (For Inhibitors and Dispersing Agents); Recent Applications in Green Chemistry

### **Further Reading**

- 1. Howard, W.L., Introduction to Industrial Chemistry, Wiley-Interscience (1986).
- 2. Weissermel, K., and Arpe, H.J., Industrial Organic Chemistry, VCH (1997) 3rd ed.
- 3. Sheldon, R.A., Arends, I., and Hannefed, U., Green Chemistry and Catalysis, Wiley-VCH Verlag GmbH and Co. (2007).
- 4. Anastas, P., and Williamson, T. C., Green Chemistry Frontiers in Benign Chemical Synthesis and Processes, Oxford University Press (1999).
- 5. Ahluwalia, V. K., and Kidwai, M., New Trends in Green Chemistry, Anamaya Publishers (2004)

### MCHL-014: CHEMISTRY LAB-IV

(02 Credits, 60 Lectures)

### **Preparation and Characterization**

**Preparations:** Synthesis and Characterization using any of UV/VIS/IR /EPR Spectral Methods and Magnetic Measurement of the following: (**Minimum Five Experiments should be Performed**)

- 1. VO (acac)<sub>2</sub>
- 2. TiO  $(C_9H_8NO)_2H_2O$
- 3. cis-K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]
- 4. Na[Cr(NH<sub>3</sub>)<sub>2</sub>(SCN)<sub>4</sub>]
- 5. Mn(acac)<sub>3</sub> (Green Method)
- 6.  $K_3[Fe(C_2O_4)_3]$
- 7. [Co(NH<sub>3</sub>)<sub>6</sub>] [Co(NO<sub>2</sub>)<sub>6</sub>]
- 8. cis-[Co(trien)  $(NO_2)_2$ ] Cl.H<sub>2</sub>O
- 9. Hg[Co(SCN)<sub>4</sub>]

- 10. [Ni(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub>
- 11. Ni(dmg)<sub>2</sub>
- 12. [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>O
- 13. cis- and trans- bisglycinatocopper(II)
- 14. Prussian Blue, Turnbull's Blue

# Further Readings:

- 1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge University Press, 1970
- 2. Synthesis and Characterisation of Inorganic Compounds, W. L. Jolly, Prentice Hall
- 3. Marr G.and B.W. Rockett. Practical Inorganic Chemistry, London: VanNostrand Reinhold Co., 1972.

MCHL-015: CHEMISTRY LAB-V (02 Credits, 60 Lectures)		
S. No.	Title of the Experiment	
1	Preparation of 1,3,5-Tribromobenzene from Aniline	
2	Preparation of 4-Nitroaniline from Aniline	
3	Preparation of Benzanilide from Benzophenone	
4	Preparation of Preparation of Anthranilic Acid from Phthalic Aci	d
5	Preparation of Preparation of <i>p</i> -Aminobenzoic Acid from Toluer	ne
6	Preparation of Preparation of Benzilic Acid from Benzaldehyde	
7	Preparation of Chalcone Epoxide from Benzaldehyde and Acetophenone	
8	Estimation of Amino Groups	
9	Estimation of Sugars	
10	Estimation of Phenol	
11	Estimation of Formaldehyde	
12	Estimation of Amino Acids	
13	Determination of Saponification Value of An Oil or Fat	
14	Determination of Iodine Value of Oil or Fat	

- 1. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
- 2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Health.
- 3. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Adward Arnold.
- 4. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
- 5. Comprehensive Practical Organic Chemistry: Preparations and Quantitative Analysis by Ahluwalia & Aggarwal, University Press.
- 6. Techniques and Experiments for Organic Chemistry by A. Ault, University Science Books.

7. Organic Analytical Chemistry, Theory and Practice, Jagmohan, Narosa Publishing House (2003)

MCHL	-016: CHEMISTRY LAB-VI	(02 Credits, 60 Lectures)	
Expt. No.	Title of the Experiment		
1	To determine the concentrations of KCI, KBr, and I	KI in a mixture by potentiometric titration.	
2	To prepare silica (or silver) nanoparticles and study	y their spectrophotometric behaviour	
3	<ul> <li>a) To synthesise metallic nanoparticles by reducir and characterise them using UV-Visible spectre</li> <li>b) To estimate the size of the nanoparticles using 3D cubic box.</li> </ul>	ometry.	
4	To determine the pKa value of methyl orange spectrophotometrically and study the effect of surfactant on it.		
5	To determine manganese/chromium in steel sample spectrophotometrically.		
6	To study the kinetics of the reaction of phenolphthalein with sodium hydroxide spectrophotometrically.		
7	To record the UV spectra of toluene and pyrimidine (any one) in methanol. Compare and discuss various transitions involved in terms of MO theory Chalcone/ Coumarin		
8	To study the spectra of mesityl oxide/ benzophenone in different solvents and classify the observed transitions in terms of $n \rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transitions. Discuss the shift in transitions relative to those in acetone by means of a qualitative MO diagram		
9	To determine the stoichiometry of the complex forr by Job's method of continuous variation and to det constant and molar absorptivity for the complex us	termine the concentration equilibrium	
10	To determine the critical micelle concentration of a conductivity method.	surfactant (sodium lauryl sulphate) by	

- 1. Experiments in Physical Chemistry, Carl W. Garland, Joseph W. Nibler, David P. Shoemaker, McGraw-Hill
- 2. Experimental Physical Chemistry, Mathews, G. Peter, Oxford Clarendon Press (1985).
- 3. Levitt, Findlay's practical physical chemistry. Longman's London:1966.
- 4. A.M. James and D.E. Pritchard. Practical physical chemistry, Longman Group Ltd: 1968.
- 5. V.D. Athawale and Parul Mathur. Experimental physical Chemistry. New Age International: New Delhi, 2001.

# Semester 3

# MCH-020: ATOMIC AND MOLECULAR SPECTROSCOPY (04 Credits, 60 Lectures)

**Fundamentals of Spectroscopy** :Recapitulating EM Radiation and its Characteristics; Role of Quantum Mechanics in Spectroscopy; Interaction of Radiation and Matter, Characteristics of Spectrum; Intensity of Signal; Boltzmann Population Distribution, Einstein Coefficients, Transition Dipole Moments and Selection Rules; Spectral Width, Natural line Width; Beer-Lambert's Law; Fourier Transform Spectroscopy, S/N Ratio

**Atomic Spectroscopy :** Hydrogen Atom Spectrum; Energy Levels and Selection Rules, Orbital and Spin Angular Momentum, Fine structure of Hydrogen Atom Spectrum, Hydrogen like Species; Multi Electron Atoms; Good Quantum Numbers, Singlet and Triplet States, Angular Momentum of Multi Electron Atoms, Spin–Orbit Coupling, Term Symbols; Zeeman and Stark Effects

**Photoelectron Spectroscopy :**Principle of Photoelectron Spectroscopy, Koopman's Theorem; X-ray Photoelectron Spectroscopy (XPS); Spin Orbit Splitting, Chemical Shift; Ultraviolet Photoelectron Spectroscopy; Applications of XPS and UPS

Rotational Spectroscopy : Rotation of Diatomic Molecules; Rigid Rotor Approximation

Determination of Bond Lengths and Atomic Masses, Isotopic Substitution, Non-Rigid Rotator; Classification of Polyatomic Molecules; Symmetric Top Molecules, Asymmetric Top Molecules; Applications of Rotational Spectroscopy

**Vibration Spectroscopy :** Vibration spectroscopy of Diatomic Molecules; Harmonic Oscillator Approximation, Force Constants And Amplitudes, Anharmonic Oscillator; Vibration-Rotation Spectra; P, Q and R Branches, Vibration Rotation Spectrum of CO; Breakdown of the Born-Oppenheimer Approximation, Interaction of Rotation and Vibration; Dissociation Energies from Vibrational Data.

**Vibrational Spectroscopy of Polyatomic Molecules (4 lectures):**Vibration Spectroscopy of Polyatomic Molecules; Normal Modes of Vibration, IR activity and Selection Rule; Overtones and Combination Bands; Effect of Rotation on Vibration Spectra; Linear Molecules, Symmetric Top

**Raman Spectroscopy :** Theory of Raman Spectroscopy; Quantum or Particle Theory, Classical or Wave Theory, Raman Activity of Vibrations, Rule of Mutual Exclusion, Depolarisation Ratio; Enhancement of Raman Spectral Intensities; Resonance Raman Spectroscopy, Coherent Anti-Stokes Raman Spectroscopy, Surface Enhanced Raman Scattering; Applications of Raman Spectroscopy

**Electronic Spectroscopy of Diatomic Molecules :** Electronic Energy Levels and Selection Rules; Molecular Term Symbols, Selection Rules; Electronic Spectrum of Diatomic Molecules; Born Oppenheimer Approximation, Vibrational Coarse Structure; Intensity of Spectral Lines, Frank Condon Principle; Rotational Fine Structure, Fortrat Diagram; Dissociation Energies of Diatomic Molecules, Birge-Sponer Extrapolation; Predissociation

**Electronic Spectroscopy of Polyatomic Molecules** :Electronic Transitions in Polyatomic Molecules; dd Transitions, Charge Transfer Transitions,  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  Transitions; Factors Affecting electronic Transitions; Chromophores and Auxochromes, Effect of Solvent, Effect of Dielectric Constant, Effect of Viscosity; Photoelectron Spectroscopy; Diatomic Molecules, Simple Polyatomic Molecule, Adiabatic and Vertical Ionization Energies; Applications of Photoelectron Spectroscopy

**Proton NMR Spectroscopy :** Basic Phenomenon of NMR; Larmour Precession and Resonance, Chemical shift, and Factors affecting it, Chemical Exchange, Spin-Spin Coupling, Spin-Spin and SpinLattice Relaxations; Nomenclature of Spin Systems; Chemical and Magnetic Equivalence, Selection Rules; Analysis of NMR Spectra; AX System, AMX System, AB System

<sup>13</sup>C and 2D NMR Spectroscopy : CW and FT-NMR; Sensitivity Issue, Pulse NMR Experiment, Fourier Transformation; <sup>13</sup>C NMR; Simplification of NMR Spectra; Homonuclear Decoupling, Heteronuclear Decoupling, Off Resonance; 2D NMR; Multi Pulse Experiment, COSY Spectrum, NOE Effect, NOESY Spectrum

**ESR Spectroscopy :** ESR Phenomenon; Electron Spin and its Characteristics, Intensity and Representation of ESR Spectrum; Hydrogen atom, Hyperfine Interaction; Isotropic Systems with More Than Two Nuclei, Contributors to Hyperfine Coupling Constants; Anisotropy in g Values; Anisotropy in Hyperfine Coupling

**Mossbauer Spectroscopy** :Mossbauer Effect, and Mossbauer Spectroscopy, Recoilless Emission and Absorption; Isomer Shift; Quadrupole Splitting; Magnetic Hyperfine Interaction

# **Further Readings**

- 1. Hollas. J. M., Modern Spectroscopy 4th Ed., John Wiley & Sons (2004).
- 2. Satyanarayana, D. N., Handbook of Molecular Spectroscopy: From radio waves to gamma rays, I.K. International Publishing House, New Delhi (2015).
- 3. Kakkar, R., Atomic & Molecular Spectroscopy, Cambridge University Press (2015).
- 4. Chang, R. Basic Principles of Spectroscopy McGraw-Hill, New York, N.Y. (1970).
- 5. Drago, Russell S. Physical Methods for Chemists 2ed. East West Press Pvt. Ltd. (2016).
- 6. C. N. Banwell and E.M. McCash, Fundamentals of MolecularSpectroscopy, TMH Edition, 2012.
- 7. G. M. Barrow, Introduction to Molecular Spectroscopy. McGraw Hill, Int. Students Edition. 1988.
- 8. J. D. Graybeal, Molecular Spectroscopy, McGraw Hill Int. StudentEdition, 1990.

# MCH-021: CHEMISTRY OF MATERIALS

(04 Credits, 60 Lectures)

**Introduction to Polymers :** Polymers and their Classification, Classification of Polymers; Tacticity of Polymers; Properties of Polymers; Crystallinity of Polymers, Glass Transition Temperature, Viscosity of Polymers; Polymer Molecular Mass; Dispersity, Determination of Molecular Mass

**Kinetics and Mechanism of Polymerisation :** Mechanism of Polymerisation; Chain Growth Polymerisation, Step growth Polymerisation, Co-polymerization; Kinetics of Addition Polymerisation; In the Absence of Catalyst, In Presence of Catalyst; Kinetics of Chain Growth Polymerisation; Free Radical Polymerization, Cationic Polymerization, Anionic Polymerization; Kinetics of Copolymerisation

**Conducting Polymers :**Conducting Polymers; Discovery of Conducting Polymers, Structural Features of Conducting Polymers, Origin of Conductivity in Conducting Polymers, Doping; Synthesis of Conducting Polymers; Electrochemical Polymerization, Chemical Polymerization, Emulsion Polymerization; Mechanism of Conduction; Band Theory, Charge Carriers (Polaron, Bipolaron, Soliton), SSH Soliton Theory, Inter-soliton Hopping Mechanism, Free-electron Molecular Orbital Model, Molecular-Electron Transfer Theory; Applications of Conducting Polymers; Biosensors, Tissue Engineering, Drug Delivery, Artificial Muscle

**Stimuli Sensitive Polymers :**Stimuli Responsive Polymers, Classification of Stimuli Responsive Polymers; pH Responsive Smart Polymers; Classification, Synthetic Strategies,

Mechanism of Action; Application of pH Sensitive Smart Polymers; Delivery of Therapeutic Agents, Biomaterials, Glucose Sensors; Temperature-Responsive Smart Polymers; Factors Affecting Temperature-Responsive Behaviour, Mechanism of Action; Stereographic Projections

**Degradable Polymers :**Polymer Degradation; Need for Polymer Degradation, Factors Causing Degradation, Changes due to Degradation, Modes of Polymer Degradation; Biodegradable Polymer; Need of Biodegradable Polymer, Mechanism of Biodegradation, Factors Affecting, Biodegradation; Chemical Degradation; Methods of Chemical Degradation, Products of Chemical Degradation; Applications of Degradable Polymers

**Hydrogels :**Introduction to Hydrogels; Classification of Hydrogels, Polymers Used in Hydrogels, Swelling Characteristics of Hydrogels; Synthesis of Hydrogels; Characterisation of Hydrogels; Biomedical Applications of Hydrogels; Stimuli Responsive Hydrogels, Glucose Sensitive Hydrogels, Hydrogels in Drug Delivery

**Functional Polymers :**Biomedical Polymers; Contact Lens, Dental Polymers; Artificial Organs; Artificial Kidney, Skin, Blood Cells; Fire-Retarding Polymers

**Biomimetic and Shape Memory Polymers :**Biomimetics; Historical Perspective, Scope of Biomimetics; Biomimetic applications; Shape Memory Polymers; Shape Memory Effect, Mechanism of Shape Memory Effect; Applications of Shape Memory polymers

**Introduction to Liquid Crystals :** Liquid Crystalline State; Characteristics of Liquid Crystals, Structural Requirements of Liquid Crystals; Classification of Liquid Crystals; Molecular arrangement in Liquid Crystals; Positional Order, Orientational Order, Bond Orientational Order; Polymorphism in Liquid Crystals, Phase Transitions

**Polymeric Liquid Crystals :**Polymeric Liquid Crystals; Main Chain Polymer Liquid Crystals, Side Chain Polymer Liquid Crystals; Ordering and Texture; Optical Properties of Liquid Crystals; Applications of Polymeric Liquid Crystals

**Surface Active Agents :** Surfactants and Their Classification; Classification of Surfactants, Hydrophilic-lipophilic Balance; Micelles; Process of Micellisation, CMC and Factors Affecting It; Thermodynamics of Micellisation; Solublisation by Surfactants, Factors Affecting Solublisation; Emulsions, Stabilisation of Macroemulsions; Surfactants at the Solid-Liquid Interface, Electrokinetic Phenomenon

**Glasses, Ceramics and Composites :** Glasses; Glassy State, Glass Formers and Glass Modifiers, Applications; Ceramics, Structure and Properties; Classification of Ceramics; Clay Products, Refractories; Composites; Classification of Composites, Formation of Composites; Applications of Glasses, Ceramics and Composites

**Nano Materials :** Introduction to Nanomaterials, Characteristics of Nano Materials; Preparation of Nanomaterials; Physical Methods, Chemical Methods; Characterisation of Nanomaterials; Electron Microscopy, Dynamic Light Scattering, Atomic Force Microscopy; Properties of Nanomaterials; Optical Properties, Electrical Properties, Mechanical Properties, Magnetic Properties; Selected Applications of Nanomaterials

**Thin and Langmuir-Blodgett Films :**Thin Films and Their Formation; Physical Methods of Film Deposition; Physical Vapour Deposition (PVD), Sputtering; Chemical Methods of Film Deposition; MOCVD, Sol-Gel; Langmuir-Blodgett (LB) Film, Properties of LB Films; Applications of Thin and LB Films

- 1. W.D. Callister, Material Science and Engineering. John Wiley & Sons; 8th Edition, 2010.
- 2. Materials Chemistry, Bradley D. Fahlman, Springer, 2011.
- 3. T. J. J. Müller and V. R. Gowariker, N. V. Viswanathan & T. Sreedhar, Polymer Science:, New Age international, 2015
- 4. H.R. Allcock and F.W. Lampe Contemporary Polymer Chemistry, Pearson/Prentice Hall, 2003
- 5. U. H. F. Bunz, Functional Organic Materials, Wiley-VCH, 2007.
- 6. Textbook of Polymer Science: F.W. Billmeyer (Wiley), 3rd Edn., 2007
- 7. Materials Chemistry, Bradley D. Fahlman, Springer, 2011
- 8. M. Srivastava and C. Srinivasan, Science of engineering materials, Wiley Eastern Ltd, 1991.
- 9. T. J. J. Müller and U. H. F. Bunz, Functional Organic Materials, Wiley-VCH, 2007.

10. György Inzelt, Conducting Polymers A New Era in Electrochemistry, Springer, 2008.

# MCH-022: SEPARATION AND SPECTROSCOPIC METHODS (04 Credits, 60 Lectures)

# Section A: Separation Methods

**Solvent Extraction :**General Principles and Terminology; Classification of Extraction Systems; Distribution of Simple Molecules, Extraction by Compound Formation, Extraction by Solvation, Extraction by Ion Pair Formation, Extraction by Crown Ethers; Diluents and Modifiers; Factors Influencing Extraction; Different Approaches for Metal Ion Separation; Criteria for the Choice of Organic Phase

**General Aspects of Chromatographic Methods** :Classification and Basic Principles; Liquid Column Chromatography; Choice of Stationary and Mobile Phases, Development Techniques; Planar Chromatography; Paper Chromatography, Thin Layer Chromatography (TLC)

**Gas Chromatography :**Basic Aspects; Instrumentation; Sampling; Introduction of Sample into GC Unit; Applications;

High Performance Liquid Chromatography : Principle; Instrumentations; Advantages; Applications

**Ion Exchange Chromatography :**Ion Exchange Mechanism; Classification of Ion Exchangers; Synthesis of Ion Exchange Resins; Trade Names and Nomenclature; Resins Properties; Synthetic Inorganic Ion Exchangers; Applications

**Size Exclusion Chromatography :**Basic Principle; Gels and Their Important Properties; Classification, Synthesis and Properties of Different Gels; Applications

**Membrane Separation :**General Aspects; Important Membrane Processes; Mechanism of Separation Through Membrane; Osmotic Phenomena and RO Process; Dialysis and Electrodialysis; Applications

**Electrophoresis** :Electroosmotic Flow; Basic Principle and Operation; Different Forms of Electrophoresis; Slab Electrophoresis; DNA Gel Electrophoresis, SDS-PAGE Gel Electrophoresis; Capillary Electrochromatography

# SECTION B: SPECTROSCOPIC METHODS

**UV-VISIBLE Spectrometry** :Origin and Characteristics of UV-VIS Spectrum; Characteristics of UV-VIS Spectrum, Absorbing Species; Principle of UV-VIS Spectrometry; Beer-Lambert's Law, Deviations from Beer-Lambert's Law; Types of UV-Visible Spectrometers; Single Beam Spectrometers Double Beam Spectrometers; Analytical Applications of UV-Visible Spectrometry; Qualitative Applications, Quantitative Applications, Quantitative Determination Methodology, Simultaneous Determination

**IR and Raman Spectrometry** :Theory of Infra-Red Spectrometry, Characteristics of IR Spectrum; Instruments for IR Spectrometry; Dispersive Infra-Red Spectrometers, Fourier Transform Infra Red Spectrometers; Applications of Infra-Red Spectrometry, Qualitative Applications, Quantitative Applications; Theory of Raman Spectroscopy; Rule of Mutual Exclusion, Depolarisation Ratio; Instrumentation for Raman Spectroscopy; Enhancement of Raman Spectral Intensities; Resonance Raman Spectroscopy, Coherent Anti-Stokes Raman Spectroscopy, Surface Enhanced Raman Scattering; Applications of Raman Spectroscopy

**Fluorimetry and Phosphorimetry :**Origin of Fluorescence and Phosphorescence Spectra; Jablonski Diagram, Fluorescent and Phosphorescent Species, Factors Affecting Fluorescence and Phosphorescence; Fluorescence Quenching, Quantum Yield; Instrumentation for Fluorescence Measurement; Instrumentation for Phosphorescence Measurement; Sampling, Recording Procedure; Applications of Fluorescence and Phosphorescence

Atomic Absorption and Emission Spectrometry :Origin and Classification of Atomic Spectra; Flame Atomic Absorption Spectrometry; Flame and its Structure, Principle of Flame Atomic Absorption Spectrometry; Graphite Furnace Atomic Absorption Spectrometry, Electrothermal Atomisers, Advantages and Disadvantages of GFAAS; Flame Atomic Emission Spectrometry; Principle of Flame Atomic Emission Spectrometry, Instrumentation for Flame Atomic Emission Spectrometry; ICP- Atomic Emission Spectrometry; Plasma and its Characteristics, Inductively Coupled Plasma, Instrumentation for ICP-AES; Interferences in Atomic Absorption and Emission Spectrometry; Interferences in AAS and GFAAS, Interferences in AES, Interferences in ICP-AES; Analytical Applications of Atomic Absorption and Emission Spectrometry

<sup>1</sup>H NMR Spectroscopy :Theory of NMR Spectroscopy; Larmor Precession, Mechanism of Resonance, Relaxation Mechanisms; Fourier Transform NMR; Chemical Shift, Factors Affecting Chemical Shift; Spin-Spin Coupling, Magnitude of Coupling Constants; Instrumentation for NMR Spectroscopy; Applications of NMR Spectroscopy; Quantitative Applications, Qualitative Applications

**Two-Dimensional NMR Spectroscopy :**Multi Pulse Technique; Two-dimensional NMR, Principle of 2D-NMR; Types of 2D-NMR Spectra, Multi Pulse Experiments; Instrumentation for 2D-NMR Spectroscopy; Analytical applications of 2D-NMR

<sup>13</sup>C NMR Spectroscopy :<sup>13</sup>C NMR; Proton decoupling, Off-Resonance Decoupling, Pulse Decoupling, Nuclear Overhauser Effect; Analytical applications of <sup>13</sup>C NMR; Structure Spectrum Correlation, Other Applications

**High Resolution Mass Spectrometry** :Theory of Mass Spectrometry; Characteristics of Mass Spectrum, Isotopic Peaks; Instrumentation for Mass Spectrometry; Ion Sources; Types of Mass Spectroscopic methods, APCI-MS, ESI-MS, MALDI-MS; Analytical applications of Mass Spectrometry; Qualitative Applications of Mass Spectrometry, Quantitative Applications of Mass Spectrometry

**Hyphenated Techniques :**Hyphenated Techniques; Spectrometer Interface, Various Types of Separators; Interfacing GC and LC with Mass Spectrometry; GC-MS, LC-MS; Interfacing GC and IR Spectrometry (GC-IR); Interfacing HPLC and Mass Spectrometry (HPLC-MS); Interfacing of Inductively Coupled Plasma and Mass Spectrometers (ICP-MS), Multielemental Character and Detection Limits; Analytical Importance of Hyphenated Techniques

**Scattering and Diffraction :**X-Rays: Generation and Properties; X-ray scattering from an Electron and an atom; Small Angle X-Ray scattering; X-ray Diffraction from a Crystal Lattice, Bragg's law; Experimental methods of X-Ray Diffraction; Applications of Scattering and Diffraction.

# **Further Readings:**

1. Christian, G. D., Analytical Chemistry, 6th Ed., John Wiley & Sons, Inc. (2004).

- 2. Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A. Principles of Instrumental Analysis Saunders Golden Sunburst Series (1997).
- 3. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) Instrumental Methods of Analysis 7th Ed., Wadsworth Publishing (1988) ISBN 0534081428
- 4. Instrumental Analysis, Editors, H.H. Bauer, G.D. Christian and J.E.O' Reilly, 2ndEdn, Allyn and Bacon, Inc., Boston (1991)
- 5. Principles and Practice of Analytical Chemistry by F.W. Fifield and D. Kealey, 5thEdn, Blackwell Science Ltd, New Delhi (2004).
- 6. Handbook of Instrumental Techniques for Analytical Chemistry, Editor, F. Settle, Low Price Edn, Pearson Education Inc, New Delhi (2004).
- 7. Instrumental Methods of Chemical Analysis by G.W. Ewing, 5thEdn, Mc-Graw Hill Singapore (1985).
- 8. Instrumental Methods of Analysis by H. H. Willard, I. L. Merritt, J. A. Dean & F. A. Seattle CBS Publishers & Distributors, New Delhi (1986).

# MCHL-017: SEPARATION AND SPECTROSCOPIC METHODS LAB (02 Credits, 60 Lectures)

Expt. No.	Title of the experiment	
1	Liquid- liquid extraction behavior of Fe (III) and Ni (II) in tri- n-butyl phosphate (TBP) from hydrochloric acid medium .	
2	Separations of Fe (III) and Ni (II) using TBP-HCI liquid- liquid extraction system.	
3	Determination of ion exchange capacity of a cation and an anion exchanger.	
4	Determination of total milliequivalents of metal ions in tap/sea water sample using a strong cation exchanger from HCI medium .	
	Or Separation of Fe (III) and Ni (II) using a strongly basic anion exchanger.	
5	Separation of cations by paper chromatography Or Separation of iron and aluminium by column chromatography .	
	Or Separation of amino acids by chromatography Or Separation of chlorophyll pigments by column chromatography	
6	Determination of Zinc in Pharmaceutical Preparations by Ion Exchange Separation and Complexometric Titration.	
7	To determine sodium and potassium <b>OR</b> calcium and magnesium in tap water by flame photometry.	
8	To determine the concentrations of Na <sup>+</sup> and K <sup>+</sup> ions flame photometrically, using internal standard method.	
9	To determine the concentrations of chromium and manganese in a mixture spectrophotometrically.	
10	The Determination of Aspirin and caffeine in a Proprietary Analgesic by Ultraviolet (UV) Spectrometry	

11	To determine the pka of an indicator spectrophotometrically.	
12	To study the Effect of pH on the visible spectrum of potassium dichromate solution.	
13	To determine the equilibrium constant of keto-enol tautomerisation reaction.	

# Further Readings:

- 1. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 2. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- 3. Findley's Practical Physical Chemistry, B. P. Levitt, Longman
- 4. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
- 5. "Principles of Instrumental Analysis" by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch, Cengage Learning
- 6. "Separation Process Principles" by J. D. Seader, Ernest J. Henley, and D. Keith Roper, Wiley
- 7. "Instrumental Methods of Analysis" by Hobart H. Willard, Lynne L. Merritt, Jr., and John A. Dean, Wadsworth Publishing
- "Introduction to Modern Liquid Chromatography" by Lloyd R. Snyder, Joseph J. Kirkland, and John W. Dolan, Wiley
- 9. "High-Performance Liquid Chromatography" by L. R. Snyder and J. J. Kirkland, Wiley
- 10. "Fundamentals of Analytical Chemistry" by Douglas A. Skoog, Donald M. West, F. James Holler, and Stanley R. Crouch, Cengage Learning

# MCH-023:: ENVIRONMENTAL CHEMISTRY

(04 Credits, 60 Lectures)

**Nature and Formation of Soil**: Soil and its Importance; Soil Morphology: Characteristics of Soil Profile, Soil Horizons; Soil Genesis: Origin and Formation of Soil: Minerals and Rocks, Weathering and Soil Formation, Factors affecting Soil Formation; Soil Classification: Soil Types of India.

**Soil Quality Parameters**: Mechanical Parameters: Soil Texture and Methods of Analysis, Soil Textural Classes, Soil Aggregation and Soil Structure, Soil Aeration, Soil Water; Biological Parameters: Soil Flora, Soil Fauna, Beneficial Role of Soil Organisms; Physico-Chemical Parameters: Crystal Structure of Clays, Ion Exchange Property of Soils, Soil pH – Acidity and Alkalinity.

**Soil Fertility and Productivity:** Plant Nutrients: Macronutrients, Micronutrients, Availability of Nutrients in Soils, Chemical Methods of Estimating Available Nutrients, Soil pH and Nutrient Availability, Soil Fertility Evaluation, Concepts in Soil Fertility, Maximum Crop Yields; Management of Soil Productivity: Fertilizers and Fertilizer Management, Factors Affecting Fertilizer Requirements, Manures, Cultural Practices.

**Water Resources**: Units for Land Area and Rainfall: Global Distribution of Water: Water Resources of India: Annual Rainfall, River Systems in Our Country, River Basins, Groundwater Availability; Hydrological Cycle: Stages in Hydrological Cycle, Abnormal Properties of Water Helping the Operations of Hydrological Cycle, Importance of Hydrological Cycle; Hydrodynamics of Fresh Water Ecosystems: Crucial Issues Associated with Conservation and Management of Water Resources: Features Related to Water Availability and Usage, Need for Conservation and Management of Water Resources; Methods of Water Conservation and Management.

**Water Characteristics**: Physical Properties of Water Systems; Chemical Properties of Water Systems; Biological Properties of Water Systems; Factors Affecting Water Quality: Natural Factors, Human Activities, Biological Transformations; Solubility of Gases in Water; Carbonate Equilibrium.

Water Quality Criteria and Uses: Concerns for Water Quality: Water Quality Criteria for Various Purposes: Objectives, Criteria and Standards – Definition, Water Quality Criteria as Basis for Classification of Water Bodies; Factors that Influence Prescription of Criteria for Water Quality; Uses of Water Quality Criteria; Monitoring and Assessment – A Discussion: Water Quality Monitoring for Water Resources Management; Water Quality Monitoring System for Risk Assessment; A Comprehensive Scheme for Controlling River Water Quality; Uses of Monitoring Programmes; Analytical Techniques for Monitoring Water Quality: Physical and Chemical Methods of Monitoring; Biomonitoring; Need for Integrated Monitoring Mechanism.

Atmosphere: Nature and Importance: Origin of Atmosphere; Regions of Atmosphere:

Regions Based on Chemical Composition, Regions Based on Temperature, Regions Based on Physical and Chemical Properties; Composition of Atmosphere: Variation of Gaseous Composition with Height, Variation of Gaseous Composition with Latitude and Season; Atmospheric Effects and Reactions: Reactions in Atmosphere; Water in Atmosphere: Water Vapour, Precipitation, Process of Precipitation ; Greenhouse Gases and Global Warming, Water Vapour, Carbon Dioxide, Methane, Nitrous Oxide, Nitrous Oxide, Chlorofluorocarbons, Ozone, Other Greenhouse Gases, Global Warming Potential of Greenhouse Gases, Energy and Greenhouse Gas Emissions; Ozone Layer and its Depletion: Effects of Ozone Layer Depletion , Ozone Layer Depletion and Global Warming, Impact of Ozone Layer Depletion on Air Pollution

**Meteorological Aspects of Air pollution:** Air Pollution Ecosystem; Primary Meteorological Parameters: Wind Speed and Wind Direction, Temperature, Atmospheric Stability, Mixing Height; Secondary Meteorological Parameters: Humidity and Precipitation, Visibility, Pressures, Solar Radiations; Influence of Stability on Stack Emissions; Meteorological Factors in Industrial Location; Urban Meteorology

**Air Pollutants:** Air Pollution Phenomenon: Air Pollutants: Common Forms; Classification of Air Pollutants: Natural and Anthropogenic Pollutants, Particulate and Gaseous Pollutants, Primary and Secondary Pollutants, Stationary and Mobile Source Pollutants, Ambient Air and Indoor Air Pollutants; Effect of Air Pollutants on Human Health: Carbon Monoxide, Nitrogen Oxides, Hydrocarbons, Sulphur Oxides, Suspended Particulate Matter; Effect of Air Pollutants on Animals: Arsenic, Fluorides, Lead, Insecticides and Pesticides;

Effect: Sulphur Dioxide, Ozone, Nitrogen Dioxide, Peroxy Acetyl Nitrate, Fluorides, Ethylene; Effect of Air Pollutants on Materials: Ferrous Metals, Aluminium and Aluminium Alloys, Copper and Silver, Building Materials, Leather, Paper, Textiles; Effect of Air Pollution on Visibility

**Air Quality monitoring and Control:** Air Quality: Indoor and Outdoor Air Quality, Air quality Management System and Standards, Measures of Air Quality; Air Quality Monitoring: National Ambient Air Management Programme, Ambient Air Sampling, Methods of Ambient Air Analysis, Analysis of Common Air Pollutants; Air Pollution Control **Industrial Effluents:** – Pollution Parameters and Treatment Methods: Pollution Parameters; Treatment Methods; Effluents from Food and Food Processing Industries – Dairy Waste: Sources of Waste; Methods for Reducing Wastewater Quantity; Treatment of Dairy Waste; Effluents from Petrochemicals: The Petrochemicals Industry; Waste Characteristics; Waste Disposal Treatment; Effluents from Textiles: The Textile Industry; Textile Waste Characteristics; Textile Wastewater Problems; Textile Waste Treatment; Effluents from Pulp and Paper Industry: The Pulp and Paper Industry; Effluent from Pulp and Paper Industry; Characteristics of Effluent; Suspended Solids Reduction; Sludge Dewatering and Disposal; Methods for the Reduction of Organics; Land Disposal by Irrigation and Seepage; Effluents from Tanneries: The Leather Industry; Tannery Waste Characteristics; Tannery Waste Treatment; Hazardous Wastes: Hazardous Waste Generation; Hazardous Waste Management.

**Environmental Pollution due to Agrochemicals:** Pesticides: Pesticides in the Environment, Effects of Pesticides in Ecosystem, Ways of Minimising Environmental Effects of Pesticides, Minimisation of Pesticides Residues, Alternative Methods of Pest Control; Environmental Pollution Due to Fertilisers: Nitrogen as Pollutant, Nitrate in Water and Food and Human Health, Nitrates and Plant Growth, Gaseous Emission, Phosphorous as Pollutant, Potassium as Pollutant, Heavy Metals as Pollutants; Strategies to Reduce Environmental Pollution due to Fertilisers: Manures as Pollutants.

**Municipal and Domestic Wastes:** Sewage and Other Water Borne Wastes: Generation and their General Characteristics, Sewage Generation, General Characteristics of Sewage, Sewage Analysis, Sewage Sampling; Solid Matters in Sewage: Determination of Solid Matters in Sewage; Organic Matters in Sewage: Carbon, Nitrogen and Sulphur Cycles in Nature, Determination of Organic Matters, Nutrients, Detergents and Surfactants, Mineral Matters in Sewage and their Determination; Gaseous and Volatile Matters in Sewage: Determination of Gases in Sewage; Hydrogen Ion Concentration and Temperature: Hydrogen Ion Concentration of Sewage, Temperature of Sewage; Living Matters in Sewage: Significance, Determination of Planktons; Microbial Contamination in Sewage: Micro-organisms in Sewage, Removal of Microorganisms, Bacteria; Decomposition of Sewage: Anaerobic Treatment of Sewage, Aerobic Treatment of Sewage, Oxygen Requirement for Decomposition of Sewage; Sewage Treatment and Disposal: Sewage Characteristics, Sewage Treatment Process, Sewage Disposal; Diseases Through Sewage.

**Effects of Soil and Water Pollution:** Industrial Pollution Cycle and Adverse Effects; Water Related Diseases; Biological Hazards, Chemical and Radioactive Hazards; Water Related Disease and Seasonal Variation: Adverse Effects of Soil Pollution: Soil Pollution of Biological Disease Agents, Soil Pollution and Solid Waste Disposal, Soil Pollution by Toxic Chemicals.

### **Further Readings:**

- 1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
- 2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
- 3. Environmental Chemistry, A. K. De, Wiley Eastern. Environmental
- 4. Environmental Chemistry, C. Baird, W. H. Freeman.
- 5. Reaction mechanisms in environmental organic chemistry, Richard A. Larson and Eric J. Weber

# MCHL-018: ENVIRONMENTAL CHEMISTRY LAB (04 Credits, 60 Lectures)

Experiment 1: i) Sampling of Soil and Water Samples

ii) Determination of pH and Conductance of Water and Soil Samples

- Experiment 2: Determination of Total Available Nitrogen in a Soil Sample
- Experiment 3: Determination of Available Phosphorus in a Soil Sample

- Experiment 4: Estimation of Alkalinity of a Water Sample
- Experiment 5: Estimation of Soluble Chlorides in a Water Sample
- Experiment 6: Estimation of Soluble Sulphates in a Water Sample
- Experiment 7: Estimation of Dissolved Oxygen in a Water Sample
- Experiment 8: Determination of Hardness in a Water Sample
- Experiment 9: Determination of Chemical Oxygen Demand of a Polluted Water Sample
- Experiment 10: Determination of Dust fall, Rainfall and Humidity
- Experiment 11: Detection of CO and NO2 in Air/ Gaseous Emissions
- Experiment 12: Determination of Suspended Particulate Matter in Air and NO<sub>2</sub> in Ambient Air/Gaseous Emissions
- Experiment 13: Determination of Sulphur Dioxide in Ambient Air/Gaseous Emission
- Experiment 14: Identification of Pesticides in Pesticide Residues

- 1. Vowels P.D. and D.W. Connel, Experiments in Environmental chemistryPergamon1980.
- 2. Pollution Analysis, S.M. Khopkar, Wiley Eastern
- 3. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
- 4. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
- 5. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern

# Semester **4**

# MCH-024: INTRODUCTION TO RESEARCH

(02 Credits, 30 Lectures)

**Foundations of Research:** Basics of Research; Meaning and Significance, Objectives of Research, Research Methods, and Research Methodology; Types of Research; Qualitative and Quantitative Research, Fundamental or Basic Research, Experimental and Non-experimental Research; Stages of Research

**Research Problem:** What is a Research Problem; Need of a Research Problem, Characteristics of a Good Research Problem, Criteria of Selecting a Research Problem; Identification of a Research Problem; Library Resources, Web Resources, Search Engine, Literature Review, Guidelines for Literature Review; Formulation of Research Problems; Framing Aim and Objectives, Research Title

**Research Design:** Definition of Research Design, Need and Importance; Features of a Good Research Design; Types of Research Design; Exploratory, Descriptive, Experimental; Research Hypotheses; Importance of Hypotheses, Characteristics of a Good Hypothesis; Types of Hypothesis; The Hypotheses Variables, Alternate versus Null Hypotheses

**Sampling and Data Analysis:** Sampling in Research; Characteristics of a Good Sample, Statistical Population; Types of samples; Data Analysis; Errors and Accuracy, Data collection Tools, Methods of Statistical Analysis

**Writing a Research Paper:** Layout of a Research Paper, Title page, Abstract, Introduction, Methodology, Results, Discussion, References; Style of writing the Scientific Report, APA/ACS format –

**Ethics in Research:** Defining Ethics in Science; Role of Ethics in Science; Terms Used in Ethics; Core Principles of Ethics; Misconduct in Academic Work; Plagiarism and Misuse of Sources, Breach of Principles; Deviations in Publishing

**Presentation of Research Work:** PowerPoint Presentation; Characteristics of a Good ppt; Use of Software (like Chemdraw, Excel, drawing tools etc); Points to Remember; Preparation of a Sample PPT with a topic of Choice

- 1. C. R. Kothari, Research Methodology Methods and Techniques, 2nd.ed. New Delhi: New Age International Publishers, 2009.
- 2. R. Panneerselvam, Research Methodology, New Delhi: PHI, 2005.
- 3. J. W. Creswell, Research Design: Qualitative, Quantitative, andMixed Methods Approaches, 3nd. ed. Sage Publications, 2008.
- 4. Kumar, Research Methodology: A Step by Step Guide for Beginners, 2nd. ed. Indian: PE, 2005.

5. B. C. Nakra and K. K. Chaudhry, Instrumentation, Measurement and Analysis, 2nd. ed. New Delhi: TMH publishing Co. Ltd., 2005.

MCH-025: ELECTROANALYTICAL TECHNIQUES AND OTHER METHODS OF ANALYSIS (04 Credits, 60 Lectures)

**Introduction to Electro Analytical Methods:** Basic Concepts; Classification and an Overview of Electroanalytical Methods; Potentiometry, Voltammetry, Polarography, Amperometry, Electrogravimetry and Coulometry, Conductometry

**Electrogravimetry:** Electrogravimetric Analysis; Polarisation; Types of Electrogravimetric Methods; Constant Current Electrolysis, Constant Cathode Potential Electrolysis, Application of Electrogravimetry

**Coulometry:** Types of Coulometric Methods; Controlled Potential Coulometry, Constant Current Coulometry; Applications of Coulometric Methods

**Voltammetry:** Electrodes and Electrode Processes; Common Voltammetric Methods; Pulse Methods, Stripping Methods; Alternating Current Methods, Determination of the nature of the ion ( $E_{1/2}$ ); Applications of Voltammetry; Voltammetry – Instrument, Practical methods: Steps Involved in Voltammetry

**Polarography:** Dropping Mercury Electrode; Currents in Polarography; Polarographic Equation; E<sub>1/2</sub>and Effect of Complexing Agents; Qualitative and Quantitative Polarographic Analysis

**Amperometric Titrations:** Basics Amperometric Titrations; Examples of Amperometric Titration; Titrations with the Rotating Platinum Electrode; Biamperometry or Dead-Stop End Point Method; Applications of AmperometricTitrations

**Thermogravimetric Analysis:** Principle; Instrumentation: Working Function of Each Component; Sources of Error in TGA; Factors Affecting TG Curve; Interpretation of TG Curve Thermogravimetric analysis (TGA); Application of Thermogravimatric Analysis; Analysis of Inorganic Mixtures, Determination of nature of Gravimetric Precipitation, Reaction Kinetics

**Differential Thermal Analysis:** Differential Thermal Method of Analysis; Principle, Instrumentation, DTA Curves, Factors Affecting DTA Curves, Sources of Errors; Applications of DTA

**Differential Scanning Calorimetry:** Differential Scanning Calorimetry; Experimental Setup, Sources of Errors, Factors Affecting DSC Curves, Interpretation of DSC Curve, Applications of DSC, Advantages of DSC; Thermometric Titrations; Principal of Thermometric Titration, Instrumentation, Application of Thermometric Titrations; Combined thermal instruments: Introduction to TGA/MS and TGA/FTIR, High Resolution TGA, Microthermal Analysis

**Fundamentals of Radioactivity:** Radioactivity and Decay Law; Natural Radioactivity; Decay Series, Classification of Nuclides, Isotopic and Relative Atomic Masses; Artificial Radioactivity; Nuclear Reactions, Commonly used Radioisotopes, Preparation of Radioisotopes and Labelled Compounds; Detection and Measurement of Radioactivity; Statistical Aspects of Radioactivity Measurements; Background in Radioactivity Measurements

**Radioanalytical Methods:** Radiotracer Techniques; Choice of Radiotracers, Factors Affecting Choice of Radiotracers; Isotope Dilution Analysis (IDA); Activation Analysis (AA); Comparison of NAA and IDA with Other Methods; Radiometric titrations (RT); Radio Chromatography (RC); Radioimmunoassay (RIA)

**Surface Analysis Methods I:** Types of Surface Measurements; Photon Probe Techniques: X-Ray Photoelectron spectroscopy; Principle, Instrumentation, Applications; Electron Probe Techniques;

Scanning Electron Microscopy (SEM):Principle, Instrumentation, Applications; Transmission Electron Microscopy (TEM); Principle, Instrumentation, Applications

**Surface Analysis Methods II:** Energy Dispersive X-ray Spectroscopy (EDX); Principle, Instrumentation, Applications; Electron Probe X-ray analysis (EPXMA); Principle, Instrumentation, Applications; Auger Electron Spectroscopy (AES); Principle, Instrumentation, Applications; Ion Probe Techniques: Rutherford Backscattering Spectrometry (RBS); Principle, Instrumentation, Applications; Secondary Ion Mass Spectrometry (SIMS) – Fundamental Aspects of Sputtering; Principle, Instrumentation (Static and Dynamic), Applications; Scanning Probe Microscopy Techniques: Scanning Tunneling Microscopy; Principle, Instrumentation, Applications; Atomic Force Microscopy; Principle, Instrumentation, Applications

### **Further Readings:**

- 1. "Electrochemical Methods: Fundamentals and Applications" by Allen J. Bard and Larry R. Faulkner, Wiley
- 2. "Instrumental Methods of Analysis" by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch, Cengage Learning
- 3. "Electroanalytical Chemistry: A Series of Advances" by Allen J. Bard, CRC Press
- 4. "Principles of Instrumental Analysis" by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch, Cengage Learning
- 5. "Modern Electrochemistry 1: Ionics" by Bockris and Reddy, Springer
- 6. "Modern Electrochemistry 2A: Fundamentals of Electrodics" by John O'M. Bockris and Amulya K.N. Reddy, Springer
- 7. "Electroanalytical Chemistry: Basic Principles and Applications" by Milan Paunović, Springer
- 8. "Electrochemical Methods of Chemical Analysis" by Fritz Scholz, Wiley

# MCHL-019: ELECTROANALYTICAL TECHNIQUES AND OTHER METHODS OF ANALYSIS LAB (02 Credits, 60 Lectures)

### List of Experiments

- 1. pH titration of a strong acid (battery acid)
- 2. pH titration of a weak acid Determination of pKa, of acetic acid
- 3. Potentiometric titration of a strong acid with a strong base using quinhydone electrode
- 4. Potentiometric titration of  $Fe^{2+}$  with  $Cr_2O_7^{2-}$
- 5. Potentiometric determination of Cl<sup>-</sup>content of common salt using AgNO<sub>3</sub>
- 6. Conductometric titration of a strong acid with a strong base
- 7. Conductometric determination of acetic acid content of vinegar
- 8. Conductometric titration of a mixture of a strong acid and weak acid with a base
- 9. Identification and determination of  $Cd^{2+}/Pb^{2+}/Zn^{2+}$  by polarography
- 10. Amperomettric titration of  $Pb^{2+}$  with  $Cr_2O_7^{2-}$
- 11. Demonstration- Determination of the solubility of a sparingly soluble salt by radiotracer method (Demo)

- 1. "Principles of Instrumental Analysis" by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch, Cengage Learning
- 2. "Experimental Electrochemistry: A Laboratory Textbook" by Oliver J. Murphy, Royal Society of Chemistry
- 3. "Instrumental Methods of Analysis" by Hobart H. Willard, Lynne L. Merritt, Jr., and John A. Dean, Wadsworth Publishing
- 4. "Electroanalytical Chemistry: Basic Principles and Applications" by Milan Paunović, Springer
- 5. "Electrochemical Methods of Chemical Analysis" by Fritz Scholz, Wiley
- 6. "Laboratory Techniques in Electroanalytical Chemistry" by Peter T. Kissinger and William R. Heineman, CRC Press

# MCHE-011- MCHE-015 ELECTIVE COURSES (TO CHOOSE ANY THREE)

# MCHE-011: APPLICATIONS OF SPECTROSCOPY TO INORGANIC & BIOINORGANIC MOLECULES (04 Credits, 60 Lectures)

**Vibrational Spectroscopy :** Vibrational Spectroscopy, Symmetry and Shapes of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>5</sub>, AB<sub>6</sub>; Mode of Bonding of Ambidentate Ligands; Ethylenediamine and Diketonato Complexes

**Application of Raman Spectroscopy :**Application of Raman Spectroscopy; Application of Resonance Raman Spectroscopy, Particularly for the Study of Active Sites of Metalloproteins

**Electron Spin Resonance Spectroscopy** :Basic Principles of ESR Inclusive of Treatment of Hydrogen Atom; ESR Spectra; Hyperfine Coupling, Organic Radicals, Transition Metal Ions; Isotropic HFS; Spin Polarization in Organic Free Radicals, Core Polarization in Transition Metal Ions; Spin-Orbit Coupling and Significance of G-Tensors and A-Tensors; Applications to Transition Metal Complexes (Having One Unpaired Electron); Biological Systems, Inorganic Free Radicals eg., PH<sub>4</sub>, F<sub>2</sub><sup>-</sup> and [BH<sub>3</sub>]<sup>-</sup>

**Applications of ESR Spectra :** Determining Charge-Delocalization in Complex Molecules, Unpaired Electron on Metal vs Unpaired Electron on Ligand; Zero-Field Splitting and Its Influence on the ESR Spectral Properties; Anisotropic (Axial And Rhombic) ESR Spectra

**NMR of Inorganic Molecules & Organometallic Compounds :**Chemical shift for Inorganic Molecules; NMR in Organometallic Compounds, Spectral Changes of Organic Ligands upon Binding to Metal Ions

**Applications of NMR Spectra in Inorganic Compounds :** Applications of NMR Spectra in Inorganic Compounds; Multinuclear NMR, <sup>1</sup>H, <sup>11</sup>B, <sup>13</sup>C -Detection and Structural Studies of Different Compounds; More Applications of NMR Spectra in Inorganic Compounds, <sup>15</sup>N, <sup>19</sup>F and <sup>31</sup>P - Detection and Structural Studies of Different Compounds

**NMR Spectral Studies in Inorganic Molecules :** NMR Spectral Studies; Tin Compounds, Vanadium Compounds, Platinum Coordinated Hydrides; Nuclear Magnetic Resonance of Paramagnetic Compounds in Solution; Variable Temperature NMR Studies; Fluxional Molecules, Exchange of Ligands; Detection of cis-trans and fac-mer Isomers

**Applications of NMR of Metal Nuclides :** The Contact and Pseudo Contact Shifts; Factors Affecting Nuclear Relaxation; Applications in Biochemical Systems; An Overview of NMR of Metal Nuclides

**Mossbauer Spectroscopy** :Mossbauer Spectral Parameters and Spectral Display; Mossbauer Effect; Basic Principles of Mossbauer Spectroscopy, Doppler Shift and Recoil Energy; Isomer Shift and its Interpretation; Nuclear Quadrupole Coupling/Splitting; Effect of Internal and External Magnetic Field on Mossbauer Spectra, Hyperfine Splitting **Applications of Mossbauer Spectroscopy-I**: Applications to Metal Complexes; Metal Carbonyls, Fe-S Cluster and Tin Compounds; Partial Quadrupole Splitting and Geometry of the Complexes

**Applications of Mossbauer Spectroscopy-II** :Applications of Mossbauer Spectroscopy; Bonding and Structures of Iron Compounds, Spin Crossover; Sn<sup>2+</sup> and Sn<sup>4+</sup> Compounds; Nature of M-L Bond, Coordination Number; Structure and Detection of Oxidation State and Inequivalent Mossbauer Atoms

**Electron Spectroscopy for Chemical Analysis (ESCA)** :Historical Background (Einstein's Photoelectric Effect, Pierre Auger, Siegbahn and coworkers, Turner and co-workers); Photoionisation and Auger Processes; Ionization Potential, Binding Energies; ESCA through UVPES and XPS, PESIS, PESOS; Meaning of Photoelectron Spectrum, Explanations in Terms of Atomic and Molecular Energy Levels

**X-Ray Fluorescence and AUGER Process** :Photoelectron Spectral Description in Terms of BE Vs Intensity, Comparison of Photoionization; X-Ray Fluorescence and AUGER Process; Related Techniques, Electron-Impact Spectroscopy, Photoemission, Penning Ionisation Spectroscopy (PIS), Ion Neutralising Spectroscopy

**AES and AAS** :Emission and Absorption Process; Atomic Spectroscopy; Spectral States for  $p^2$  and  $d^2$ Electronic Configurations (Example), Concentration Determination for Impurities in Solid State and Metal Ions in Biological Materials; Characteristic Emission or Absorption for Individual Elements; Modern Day Instrumentation

# **Further Readings:**

- 1. "Spectroscopic Methods in Inorganic Chemistry" by Ralf W. Adams, CRC Press
- 2. "Inorganic Spectroscopic Methods" by Alan K. Brisdon, Oxford University Press
- 3. "Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life" by Ivano Bertini, Harry B. Gray, Edward I. Stiefel, and Joan S. Valentine, University Science Books
- 4. "Spectroscopic Properties of Inorganic and Organometallic Compounds: Techniques, Materials, and Applications" by Joseph R. Lakowicz, Wiley
- 5. "Inorganic Spectroscopy" by A. B. P. Lever, Elsevier
- 6. "Inorganic Electronic Structure and Spectroscopy: Methodology" by Edward I. Solomon, David R. Larson, and James A. Ibers, Wiley
- 7. "Bioinorganic Chemistry" by Stephen J. Lippard and Jeremy M. Berg, University Science Books
- 8. "Bioinorganic Chemistry: Structure and Bonding" by Wolfgang Kaim and Brigitte Schwederski, Springer
- 9. "Biological Inorganic Chemistry: A New Introduction to Molecular Structure and Function" by Robert R. Crichton, Academic Press
- 10. "Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life" by Wolfgang Kaim and Brigitte Schwederski, Wiley

# MCHE-012: SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS (04 Credits, 60 Lectures)

**UV-Visible Spectroscopy: Some Basic Concepts :**Various Electronic Transitions; Beer-Lambert Law; Effect of Solvent on Electronic Transitions; Ultraviolet Spectra of Carbonyl Compounds; Unsaturated Carbonyl Compounds

**UV-Visible Spectra of Some Illustrative Compounds :**Ultraviolet Spectra of Dienes; Conjugated Polyenes; Fieser-Woodward Rules for Conjugated Dienes and Carbonyl Compounds; Ultraviolet Spectra

of Polyenes; Ultraviolet Spectra of Aromatic Compounds; Steric Effect in Biphenyls

**Infrared Spectroscopy-Basic Aspects and Applications :**Instrumentation and Sample Handling; Characteristic Vibrational Frequencies of Alkanes, Alkenes, Alkynes and Aromatic Compounds; IR Spectra of Alcohols, Phenols and Ethers; IR Spectra of Amines

**IR Spectra of Some More Classes of Organic Compounds :** IR Spectral Study of Vibrational Frequencies of Carbonyl Compounds: Aldehydes and Ketones; Carboxylic Acids, Derivatives of Carboxylic Acids, Esters, Amides, Anhydrides; IR Spectra of Lactones, and Lactams; IR Spectra of Conjugated Carbonyl Compounds; Effect of Hydrogen Bonding and Solvent Effect on Vibrational Frequencies; Overtones, Combination Bands and Fermi Resonance

**Basic Concepts of NMR Spectroscopy :**Natural Abundance of <sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P Nuclei; The Spinning Nucleus; Effect of External Magnetic Field; Processional Motion and Frequency; Energy Transitions

<sup>1</sup>H NMR Spectroscopy :Chemical Shift and Its Measurement; Factors Influencing Chemical Shift; Anisotropic Effect, Electronegativity/Inductive Effect, Hybridisation, Hydrogen Bonding; Chemical and Magnetic Equivalence; Spin-Spin Coupling; Magnitude of Coupling Constants; Simple, Virtual and Complex Spin-Spin Coupling; Factors Affecting the Coupling – First and Non-First Order Spectra; Proton Exchange

**Complex NMR Spectra :**Simplification of Complex Spectra; Solvent Effect, Field Effect; Double Resonance and Lanthanide Shift Reagents; NOE Experiments, (NOESY, HOESY, ROESY, etc.)

**Applications of NMR Spectroscopy :**Structure Elucidation of Simple Organic Compounds, Structure Elucidation of Some Complex Organic Compounds; Applications of NMR Spectroscopy in Medicine and Diagnosis; Applications of NMR Spectroscopy in Poymers; Solid-state NMR Spectroscopy; We may add some more applications

**Introduction to 2D-NMR:** Basics of COSY and its Application; Basics of HMQC and its Application; HETECOR Spectra and its Application;

<sup>13</sup>CNMR Spectroscopy : Resolution and Multiplicity of <sup>13</sup>CNMR; <sup>1</sup>H-decoupling; Noise Decoupling, Broad Band Decoupling, Off-resonance Decoupling; Deuterium, Fluorine and Phosphorus Coupling; NOE Signal Enhancement; DEPT and INEPT

**Applications of DEPT, INEPT and <sup>13</sup>CNMR Spectroscopy :** Structural Applications of; DEPT, INEPT, CMR Studies

**MASS Spectrometry :** Theory and Instrumentation; Unit Mass and Molecular Ions; Important Terms-(Singly, Doubly/Multiple Charged Ions, Metastable Peak, Base Peak, Isotopic Mass Peaks, Relative Intensity, FTMS, etc. ); Recognition of M<sup>+</sup> Ion Peak; Ionisation Methods (EI, CI, FAB, ESI, APCI and MALDI)

**General Fragmentation Rules :** Fragmentation of Oxygen Containing Organic Compounds; Fragmentation of Sulphur Containing Organic Compounds; Fragmentation of Nitrogen and Halogens Containing Organic Compounds;  $\alpha$ -,  $\beta$ -, Allylic and Benzylic Cleavages; Mc Lafferty Rearrangement; Ortho Effect

Structure Elucidation of Organic Compounds using IR, NMR and Mass Spectra : Examples of Structure Elucidation of Different Compounds

- 1. Introduction to Spectroscopy by Donald L. Pavia, Gary M. Lampman and George S. Kriz
- 2. "Spectrometric Identification of Organic Compounds" by Robert M. Silverstein and Francis X. Webster, Wiley

- 3. "Introduction to Spectroscopy" by Pavia, Lampman, and Kriz, Cengage Learning
- 4. "Structure Elucidation by NMR in Organic Chemistry: A Practical Guide" by Eberhard Breitmaier and Gunther Jung, Wiley-VCH
- 5. "Organic Spectroscopy" by William Kemp, Palgrave Macmillan
- 6. "Spectroscopic Methods in Organic Chemistry" by Dudley H. Williams and Ian Fleming, McGraw-Hill Education
- 7. "Mass Spectrometry for the Novice" by John Greaves and Andrew Bradbury, CRC Press
- 8. "Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications, and Experimental Methods" by Joseph B. Lambert, Herbert P. Oneil, and David Haas, Pearson
- 9. "Spectroscopy of Organic Compounds" by P.S. Kalsi, New Age International

# MCHE-013: SUPRAMOLECULAR CHEMISTRY (04 Credits, 60 Lectures)

**Concepts of Supramolecular Chemistry (4 hrs):** Supramolecular Chemistry, Definition and Development; Nature of Supramolecular Interactions, Ion-ion, ion-dipole, dipole-dipole, H-bonding, van der Waals and Solvophobic Interactions

**Different Effects and Binding Processes (4 hrs):** Cooperativity, Anti-cooperativity and Allosteric Effects, Induced Fit; Kinetically Controlled and Thermodynamically Controlled Binding Processes, Complexation Selectivity

**Molecular Receptors (4 hrs):** Design of Molecular Receptors, Chelate Effect ; Preorganization, Enthalpy and Entropic Contributions

**Molecular Recognition (5 hrs):** Molecular Recognition; Types of Recognition, Classification of Host Guest Compounds, Cation Binding Hosts, Binding of Anions, Neutral Molecules, Organic Molecules

**Cation-binding Hosts (4hrs):** Concepts; Cation Receptors; Crown Ethers, Cryptands, Spherands, Calixarens; Selectivity of Cation Complexation, Macrocyclic and Template Effects

Binding of Anions (4 hrs): Concepts, Anion Host Design; Anion Receptors, Shape and Selectivity

**Binding of Neutral Molecules (4 hrs):** Neutral Receptors; Clathrates, Cavitands, Cyclodextrins, Cyclophanes

**Supramolecular Chemistry in Biology I (5 hrs):** Self-Replication as the Key to Life, Replicators and Replicator Evolution, Orthogonal Translation; Origin of Life, Compartmentalization, Catalysis and Replication

**Supramolecular Chemistry in Biology II (4 hrs):** Cells, Membranes; Photosynthesis and Artificial Leaves, Oxygen Transport; Biological Mimics; Enzymes, Metallobiosites, Heme Analogues

**Supramolecular Catalysis and Transport (4 hrs):** Supramolecular Reactivity and Catalysis; Transport Processes and Carrier Design

**Self-assembly (5 hrs):** Biological Self Assembly, The Tobacco Mosaic Virus and DNA; Self-Assembling Coordination Compounds; Molecular Squares, Boxes and Spheres, Self-Assembly of Metal Arrays; Supramolecular Entanglements, Rotaxanes, Catenanes and Knots

**Solid-state Supramolecular Chemistry (4 hrs):** Solid State Inclusion Compounds, Clathrate Formation; Tectons, Synthons, Co-crystals; Polymorphism

**Supramolecular Devices** (4 hrs): Supramolecular Photochemistry; Supramolecular Electronic Ionic and Switching Devices; Self-assembly in Supramolecular Chemistry, Examples

**Applications of Supramolecular Chemistry (5 hrs):** Rational Design; Molecular Paneling; Supramolecular Devices; Nanoscience Applications

### Further Reading:

- 1. J. M. Lehn, Supramolecular Chemistry, Concepts and Perspectives, VCH, 1995.
- 2. H. Dodziuk, Introduction to Supramolecular Chemistry, Kluwer Academic, 2002.
- 3. F. Vogtle, Supramolecular Chemistry, An Introduction, John Wiley & Sons, 1991.
- 4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, A Concise Introduction, John Wiley, 2000.
- 5. A. Bianchi, K. B. James, E. G. Espana, Supramolecular Chemistry of Anions, Wiley-VCH, 1997.
- 6. M. Fujita, Molecular Self-assembly, Organic Versus Inorganic Approaches, Springer, 2000.
- 7. J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vogtle, J. M. Lehn, Comprehensive Supramolecular Chemistry, Pergamon, 1996.

# MCHE-014: PRIMARY AND SECONDARY METABOLITES (04 Credits, 60 Lectures)

**Basic Aspects of Terpenes:** Occurrence; Isolation; Classification; Nomenclature; Structure Determination; General Methods of Structure Determination, Isoprene Rule

**Synthesis of Monoterpenes:** Biosynthesis and Synthesis of the Following Monoterpenoids; Citral, Geraniol, *α*-terpeneol, Menthol

**Sesquiterpenoids:** Chemistry and Synthesis of Farnesol (Acyclic); Chemistry and Synthesis of Zingiberene (Monocyclic); Chemistry and Synthesis of Santonin (Bicyclic)

Diterpenoids: Biosynthesis and Synthesis of Phytol; Biosynthesis and Synthesis of Abietic Acid

General Methods of Structure Determination of Carotenes:  $\beta$ -carotene;  $\alpha$ - carotene;  $\gamma$ -carotene; Lycopene and Vitamin A

**Xanthophylls:** Spirilloxanthin; Capsorubin; Fucoxanthin; Carotenoid Acids (Apocarotenoids): Bixin and Crocetin; Bio Synthesis of Carotenoids

Basic Aspects of Alkaloids: Occurrence; Isolation; Nomenclature; Physiological Action

**Structural Aspects of Alkaloids:** General Methods of Structure Elucidation; Degradation; Classification Based on Nitrogen Heterocyclic Ring; Role of Alkaloids in Plants

**Structure, Synthesis and Biosynthesis of Alkaloids:** Ephedrine; Coniine; Nicotine; Atropine; Quinine; Morphine

**Basic Aspects of Steroids:** Occurrence; Nomenclature; Basic Skeleton; Diel's Hydrocarbon and Stereochemistry

Cholesterol: Isolation; Structure Determination; Synthesis of Cholesterol

Chemistry of Steroids: Androsterone; Testosterone; Estrone; Progestrone; Biosynthesis of Steroids

Some Basic Aspects: Occurrence; Nomenclature; General Methods of Structure Determination

**Anthocyanins:** Occurrence, Isolation and Synthesis of Cyanin; Occurrence, Isolation and Synthesis of Pelargonidin; Chemistry of Hirsutidin

**Polyphenols-I:** Occurrence and Synthesis of Flavones (Chrysin); Occurrence and Synthesis of Flavonols (Quercitin); Occurrence and Synthesis of Isoflavones (Daidzein)

**Polyphenols-II:** Occurrence and Synthesis of Coumarins; Occurrence and Synthesis of Quinones (Lapachol); Biosynthesis of Flavonoids: Acetate Pathway and Shikimic Acid Pathway

### **Further Readings:**

- 1. Natural Products- Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex.
- 2. Organic Chemistry Vol. II, I.L. Finar, ELBS.
- 3. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 4. Introduction to Flavonoids, B.A.Bohm, Harwood Academic Publishers.
- 5. New Trends in Natural Product Chemistry, Atta-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.

# MCHE-015: ADVANCED KINETICS AND ELECTROCHEMISTRY (04 Credits, 60 Lectures)

**Kinetics of Complex Reactions** Reversible Reactions, Opposing reactions of Second Order; Parallel Reactions; Consecutive Reactions; Autocatalysis, Steady-State Treatment

**Kinetics of Photochemical Reactions :**Photochemical Reactions, Kinetic Features of Photochemical Reactions; Kinetics of Chain Reactions; Hydrogen-Chlorine Reaction, Hydrogen- bromine Reaction, Pyrolysis of Acetaldehyde

**Kinetics of Oscillatory Reactions :**Oscillatory Reactions: Historical Account; Models of Chemical Oscillations, Lotka-Volterra Model; Belousov-Zhabotinskii Reaction, Mechanism of B-Z Reaction; Briggs-Rauscher Reaction

**Kinetics of Solid State Reactions :**Characteristics of Solid-State Reactions, Factors Affecting Solid State Reactions; Wagner's Mechanism ; Rate laws for Solid State Reactions

**Electron Transfer Reactions :**Inner Sphere Electron Transfer; Taube's Experiments, Characteristics of inner Sphere Electron Transfer Reactions, Mechanism of Inner Sphere Electron Transfer Reactions; Outer Sphere Electron Transfer, Marcus Theory

**Complex Enzyme Reactions :** Michaelis-Menten Mechanism; Reactions with Single Intermediate, Reactions with Double Intermediates; King-Altman Method, Complex Enzyme Reactions; Enzyme Inhibition, Reversibility and Products Inhibition.

**Reaction Dynamics :**Molecular Reaction Dynamics, Energy Disposal in an Exoergic Chemical Reaction; Molecular Beams, Principle of Crossed-Molecular Beams; Molecular Collisions; Impact Parameter, Collision Cross-ection, Reaction Cross-section; Reaction Cross-section and Reaction Rate

**Electrode Kinetics** :Essentials of Electrode Reactions; Butler-Volmer Equation; Derivation of Equation, Significance of Butler-Volmer Equation; Overpotential; Current-Overpotential Equation, Tafel Plot

**Kinetics of Multistep Electrode Reactions :**Multistep Electrode Reaction Pathway, Rate Determining Step; Two-Step Electrochemical Reactions; Complex Electrochemical Reactions; Charge Transfer at Electrode-Solution Interfaces; Quantization of Charge Transfer, Tunnelling

**Electrochemical Methods :** Coulometry; Controlled Potential Coulometry, Controlled Current Coulometry; Hydrodynamic Techniques; The Dropping Mercury Electrode, The Rotating Disc and Ring Disc Electrode; Scanning Probe Microscopy; Electrochemical Instrumentations

**Corrosion :** Introduction to Corrosion, Forms of Corrosion; Electrochemical Corrosion Theory, Corrosion Cells and Reactions; Corrosion Monitoring, Factors Affecting the Rate of Corrosion; Prevention of Corrosion; Metallic Coating, Electrical Protection, Corrosion Inhibitors, Impressed Current Cathodic Protection (ICCP)

**Conversion And Storage of Electrochemical Energy :** Fuel Cells; Charge Distribution around Central Ion, Chemical Potential Changes due to Ion-Ion Interactions; Supercapacitors; Classification of

Supercapacitors, Supercapacitors versus Batteries, Electrochemical Double-Layer Capacitors, Hybrid Capacitors; Applications of Supercapacitors; Lithium-Ion Batteries, Advantages and Disadvantages of Lithium-Ion Batteries

**Electrocatalysis :** Electrocatalysis; Sabatier Principle, Factors Affecting Electrocatalysis; Applications of Electrocatalysis; The Hydrogen Evolution Reaction (HER), The Carbon Dioxide Reduction Reaction

**Electrocrystallisation :**Electro Growth of Metals on Electrode; Nucleation, Growth, Surface Diffusion; Underpotential Deposition; Mechanism of UPD, Characteristics of UPD; Shapes Formed in Electrodeposition

- 1. "Physical Chemistry: A Molecular Approach" by Donald A. McQuarrie and John D. Simon; University Science Books
- 2. "Modern Electrochemistry 2A: Fundamentals of Electrodics" by John O'M. Bockris and Amulya K.N. Reddy, Springer
- 3. "Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology, and Environmental Science" by John O'M. Bockris and Amulya K.N. Reddy, Springer
- 4. "Electrochemical Methods: Fundamentals and Applications" by Allen J. Bard and Larry R. Faulkner, Wiley
- 5. "Electrochemical Reaction Engineering" by Andrzej Lasia, Springer
- 6. "Principles of Chemical Kinetics" by James E. House, Academic Press
- 7. "Kinetics of Chemical Reactions: Decoding the Concepts and Clarifying the Language" by Alexandru T. Balaban, Springer
- 8. "Physical Chemistry" by Peter Atkins and Julio de Paula, Oxford University Press