

# **Semester-II**

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Core Course**  
**Course Title: Metal Clusters and Electronic Spectra of Metal Complexes**  
**Course Code: PCH-CC-201**

Credits = 4

M.M. =

100 (70+30)

**Unit-I: Pi-Acid Complexes**

Metal carbonyls, Structure and bonding, Dative overlap, Backbonding ( $\pi\pi$ - $d\pi$ ) synergic interaction, Vibrational spectra of metal carbonyls for bonding and structural elucidation, Important reactions of metal carbonyls, Identification of isomers, IR active bands, Preparation, Bonding, Structure and important reactions of transition metal nitrosyl. Structure of rousins red and rousins black. Nature of M-NO bond, Dinitrogen and dioxygen complexes, Bonding scheme.

**Unit-II: Metal Clusters**

Occurrence of metal-metal bonds. Structure of some carbonyl metallocenes. (1) Polynuclear compounds (2) Lower halides and oxides. (3) Pre-requisites for the formation of metal-metal bond. (4) Trinuclear compounds (5) Tetranuclear clusters, Metal only clusters. Bonding in metal clusters. Metal carbonyl and metal carbonyl halide clusters, Compounds with metal-metal multiple bonds. Structure and bonding.

**Unit-III: Electronic Spectra and Magnetic Properties of Transition Metal Complexes**

Spectroscopic ground states, Correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states), Calculations of  $Dq$ ,  $B$  and  $\beta$  parameters, Charge transfer spectra, Types of magnetic bodies, orbital and spin effect, Curie equation and Curie Wies law, Determination of magnetic susceptibility, Quenching of orbital concentration, Anomalous magnetic moments, Magnetic exchange coupling and spin crossover.

**Unit IV: Symmetry and Group theory**

Symmetry elements and operations, Combination of symmetry operations, Groups, Subgroups, Classes, Group multiplication tables, Symmetry point groups, Identification of point groups, Systematic procedure for assignment of point groups to molecules, Symmetry classes and their geometrical significance, Character table ( $C_{2v}$ ,  $C_{3v}$ ).

**Books Recommended:**

- Symmetry and Spectroscopy of Molecules, K. Veera Reddy, 2<sup>nd</sup> Edn.; 2009
- Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 3<sup>rd</sup> Edn.; 2009
- Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4<sup>th</sup> Edn.; 2008.
- Comprehensive Coordination Chemistry G. Wilkinson, R. D. Gillars and J. A. M. Clevert, 2<sup>nd</sup> Edn.; 2003.
- Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, John Wiley 6<sup>th</sup> Edn.; 1999.
- Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London, 1<sup>st</sup> Edn.; 1998
- Chemistry of the Elements, N. N. Greenwood and A. Earnshaw, Pergamon. 2<sup>nd</sup> Edn.; 1997
- Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier. 2<sup>nd</sup> Edn.; 1997
- Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons, 1997
- Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series, 1<sup>st</sup> Edn.; 1991.
- Chemical Applications of Group Theory, F. A. Cotton, Wiley NY, 3<sup>rd</sup> Edn.; 1990
- Magnetochemistry, R. L. Carlin, Springer Verlag, 1986

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Core Course**  
**Course Title: Mechanism of Organic Reactions**  
**Course Code: PCH-CC-202**

Credits = 4  
M.M. = 100 (70+30)

**Unit-I: Substitution Reactions:**

**Review and recapitulation of:** Aliphatic nucleophilic:  $S_N1$ ,  $S_N2$ , Walden inversion, Mixed  $S_N1$ ,  $S_N2$ ,  $S_NI$  and SET mechanisms, Effect of leaving group and solvent. Substitution at allylic, benzylic and vinylic carbon atoms.

Aliphatic electrophilic: Mechanisms of reactions involving migration of double bond, Effect of substrate, Leaving group and solvent polarity on reactivity.

Aromatic electrophilic: The Arenium ion mechanism, Energy profile diagrams, Ipso attack, Vilsmeier, Gatterman-Koch, Reimer-Tiemann reactions, Diazonium coupling.

Aromatic nucleophilic: Introduction to different mechanisms of aromatic nucleophilic substitution,  $S_NAr$ .

Free radical substitution: Types and mechanism, Neighbouring group assistance, reactivity in attacking radicals, effect of solvent on reactivity. Allylic and alkyl halogenation, Auto-oxidation, Coupling of alkynes and diazonium salts, Sandmeyer reaction, Hunsdiecker reaction

**Unit-II: Elimination Reactions**

**Elimination reactions:** The  $E_1$ ,  $E_2$  and  $E_{1CB}$  mechanisms and orientation of the double bond. Saytzeff and Hoffman's rule. Effect of substrate structure, attacking base, leaving group and medium.

Mechanistic insights of some elimination reactions: Hydro-alkoxy-elimination, *epi*-oxy-elimination, Chugaev elimination, Hoffman elimination, Cope's elimination, Shapiro reaction, Bamford-Stevens reaction, Corey-Winter reaction, Ramberg-Bamford reaction, Boord reaction.

**Unit-III: Addition reactions**

**Addition to carbon-carbon multiple bond:** Addition reaction involving electrophiles, (Markownikoff's rule, Peroxide effect), nucleophiles and free radicals, Addition to cyclopropanes, Hydrogenation of double bond and triple bonds. Hydrogenation of aromatic rings, Hydroboration, Michael addition.

**Addition to carbon-hetero multiple bonds:** Overview of reactive carbonyl compounds, Mechanisms of addition of  $H_2O$ , HCN, Alcohols, Amines, Addition of Hydrazine, Hydrides to aldehydes and ketones. Mechanism of Wittig, Mannich, Aldol, Cross Aldol, Cannizzaro, Knoevenagel, Robinson annulation, Claisen, Dieckman, Benzoin, Perkin and Stobbe's reactions.

**Unit-IV: Molecular Rearrangement Reactions**

Classification and General mechanistic treatment of electrophilic, nucleophilic and free radical molecular rearrangement. Mechanism of the following rearrangement: Wagner-Meerwein, Pinacol-Pinacolone, Demjanov ring contraction and ring expansion, Benzil-benzilic acid, Favorski, Wolff, Neber, Hoffman, Curtius, Lossen, Schmidt, Beckmann, Baeyer-Villiger, Stevens, Wittig, Claisen, Benzidine, Brook and Wallach rearrangements.

**Books Recommended:**

- Fundamentals of Organic Chemistry; Solomons; Wiley; 12<sup>th</sup> Edn.; 2015.
- Organic Chemistry, John McMurry; Brooks/Cole; 9<sup>th</sup> Edn.; 2015
- Advanced Organic Chemistry, Reactions, Mechanism and Structure, Jerry March, 7<sup>th</sup> Edn.; 2013.
- Advanced Organic Chemistry; 5<sup>th</sup> edn.; F. A. Carey and R. J. Sundberg; Springer Plenum; 2007.
- Organic Chemistry; J. Hornback; Brooks/Cole; 2<sup>nd</sup> Edn.; 2005.

- Structure and Mechanism in Organic Chemistry; C. K. Ingold; CBS; 2<sup>nd</sup> Edn.; 2000.
- Reaction Mechanism in Organic Chemistry; S. M. Mukherjee and S. P. Singh; Macmillan; 3<sup>rd</sup> Edn.; 1998.
- A Guide Book to Mechanism in Organic Chemistry; Peter Sykes; Longman; 6<sup>th</sup> Edn.; 1996

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Core Course**  
**Course Title: Quantum Chemistry & Electrochemistry**  
**Course Code: PCH-CC-203**

Credits = 4  
M.M. = 100 (70+30)

**Unit-I: Quantum Chemistry-III**

Variation theorem, Linear variation principle, Application to Hydrogen atom and Helium atom, Perturbation theory- first order (non-degenerate & degenerate), Application of perturbation method to Helium atom, Chemical bonding, LCAO-MO approximation,  $H_2^+$  molecular ion, Brief introduction to  $H_2$ , Molecular term symbols, Valence bond treatment of  $H_2$ , Comparison of MO and VB methods in the light of  $H_2$  molecule, Hybridization of orbitals ( $sp$ ,  $sp^2$  &  $sp^3$ ).

**Unit-II: Quantum Chemistry-IV**

Huckel's Pi-MO theory, Application to linear and cyclic polyenes, Pi-electron charge and bond-order. Alternant hydrocarbons, Naphthalene, Heteroatomic conjugated systems. Limitations of Huckel theory, Parisar-Parr-Pople method and extended huckel-method (basic idea), Self-Consistent field method: Hamiltonian and wave function for multi-electron systems, Electronic hamiltonian, Antisymmetrized wave function, Slater-determinant, Hartree-Fock self-consistent field method in the light of system one and two electron integrals.

**Unit-I: Electrochemistry-I**

Ion-solvent Interactions: Non-Structural (Born) treatment and an introduction to structural (Ion-Dipole, Ion-Quadruple) treatments of ion-solvent interactions, Ion-Ion interactions: Activity and activity coefficients, Debye-Huckel theory of activity coefficients of electrolyte solutions; Derivation of Debye-Huckel limiting law, Validity and extension to high concentrations, Ion-pair formation- Bjerrum model, Debye-Huckel-Onsager conductance equation and brief idea of its extension.

**Unit-II: Electrochemistry-II**

Metal-electrolyte electrified interfaces, Concept of surface excess, Thermodynamics of electrified interface, Lippmann equation, Electrocapillary curves, Methods for determination of surface excess. Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, Recent advances. Semiconductor electrodes: Structure of semiconductor/electrolyte interface, Theories of heterogeneous electron transfer: Electron transfer at electrified interface at and away from equilibrium, Butler-Volmer Equation, Low and high field approximations, Significance of transference-coefficient.

**Books Recommended:**

- Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7<sup>th</sup> Edn.; 2013.
- Molecular Electronic-structure Theory, Helgaker et al., 2013
- Quantum Chemistry, Prasad, New Age Publishers, 4<sup>th</sup> Edn.; 2010 (Reprint 2014).
- Molecular Quantum Mechanics- P. W. Atkins and R. S. Friedmann, Oxford, 5<sup>th</sup> Edn.; 2010.
- Chemical Kinetics, K. J. Laidler, Mcgraw-Hill, 4<sup>th</sup> Edn.; Revised, 2002
- Chemical Kinetics and Catalysis, R. I. Masel, Wiley, 2001.
- Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W. L. Hase, 2<sup>nd</sup> Edn.; 1998.
- Introductory Quantum chemistry- A. K. Chandra, Tata McGraw Hill, 1998.
- Methods of Molecular Quantum Mechanics, R. Mc Weeny, Academic Press, 2<sup>nd</sup> Edn.; 1992.
- Coulson's Valence, R. Mc Weeny, ELBS, 3<sup>rd</sup> Edn.; 1980.

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Discipline Centric**  
**Course Title: Chromatographic Techniques**  
**Course Code: PCH-DCE-204**

Credits = 3  
M.M. = 100 (70+30)

**Unit-I: Thin-Layer Chromatography**

Introduction and principle, Types and selection of stationary phases (adsorbents) and mobile Phases, Methods of plate development; Detection of spots; Performance characteristics of Thin-Layer plates, Retardation and retention factor, Plate heights, High-performance thin-layer chromatography, Application  
Chiral chromatography: Chiral derivatization, Chiral mobile-phase, Chiral stationary phases, Mechanism of chiral interactions, Applications.

**Unit-II: Size Exclusion and Ion Exchange Chromatography**

Introduction and principle, Gels, Theoretical basis, Exclusion limit, Total permeation and selective permeation regions. Relation between elution volume and molecular weight, Fractionation in a complex mixture, Packing materials and applications,  
Introduction to ion-exchange chromatography, Types of ion exchange materials, Mechanism of ion exchange, Ion exchange equilibrium, Volume and ion exchange capacity, Ion chromatography. Distinction between ion-exchange and ion chromatography, Applications IEC for separation of biological molecules.

**Unit-III: High Performance Liquid Chromatography (HPLC)**

Introduction; Principle, Theory and instrumentation, Plate theory, Rate theory, Van-Deemter-Equation, Resolution, Retention time and other basic parameters, Basic difference between HPLC and conventional liquid-chromatography, Packing materials and equipments, Detectors, Advantages and Applications, Reverse phase HPLC and normal phase HPLC, Brief Introduction to hyphenated LC-MS technique.

**Unit-IV: Gas Chromatography**

Introduction and principle, Instrumentation: Columns and stationary phases, Detectors:- TCD, FID and Electron Capture Detector, Factors Affecting the efficiency of the column, Van-Deemter Equation, Qualitative and quantitative analysis based on peak height and peak area, Brief introduction to hyphenated GC-MS technique.

**Books Recommended:**

- Analytical Chemistry by G. D. Christian, John Wiley & Sons Inc, Singapore., 7<sup>th</sup> Edn.; 2013.
- Gas Chromatography and Mass Spectrometry: A Practical Guide, O David Sparkman, Zeldia Penton and Fulton G. Kitson, Elsevier, 2<sup>nd</sup> Edn.; 2011.
- Introduction to Modern Liquid Chromatography: L. R. Snyder & J. J. Kirkland (John Wiley & Sons, New York). 3<sup>rd</sup> Edn.; 2009
- Chromatography: Concepts and Contrasts, James M. Miller, Wiley, 2<sup>nd</sup> Edn.; 2009.
- Principles of Instrumental Analysis, Skoog, Holler, Nieman, 6<sup>th</sup> Edn.; 2006
- Principles and Practice of Analytical Chemistry by F. W. Fifield and D. Kealey, Blackwell Science Ltd, New Delhi 5<sup>th</sup> Edn.; 2004.
- Handbook of Instrumental Techniques for Analytical Chemistry, Editor, F. Settle, Pearson Education Inc, New Delhi. Low Price Edn, 2004.
- Instrumental Methods of Analysis, Willard, Merit, Dean and Settle, CBS Publishers and Distributors, 7<sup>th</sup> Edn.; 2004.
- Chiral Separations by liquid chromatography and related technologies, Hassan Y. Aboul-Enein, Imran Ali, CRC press, 2003.
- Chromatography and Separation Science By Satinder Ahuja McGraw Hill Pub, 5<sup>th</sup> Edn.; 1985.
- Chromatographic Methods by A. Braithwaite and F.J. Smith by Kluwer Academic Publishers 5<sup>th</sup> Edn.; 1999

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Discipline Centric**  
**Course Title: Bioinorganic Chemistry**  
**Course Code: PCH-DCE-205**

Credits = 3

M.M. =

100 (70+30)

**Unit-I: Metal ions in Biochemical Systems**

Introduction to bio-inorganic chemistry, Concept of essentiality, Criteria and classification of essential elements as per their role in living systems, Bulk metals and trace metals, Role of alkali and alkaline earth metals in biosystems, Metal ion toxicity,  $\text{Na}^+$ - $\text{K}^+$  pump, Biochemistry of iron (transport and storage), Application of radioactive elements for biosystems.

**Unit-II: Metalloporphyrins and Respiration**

Metalloporphyrins, Cytochromes (Cytochromes C, Cytochrome C-oxidase, Cytochrome P-450). Dioxygen transport (haemocyanin and hemoerythrin), Structure and physiological role of hemoglobin and myoglobin, Bohr Effect and cooperativity, Chloride effect.

**Unit-III: Electron Transport in Biosystems**

Electron transport in biosystems, Iron-Sulfur proteins, Ferredoxins, Rubredoxin, Blue copper proteins, Photosynthesis (PS I and PS II), Z-scheme, Structure of chlorophyll a and b, Manganese complex, Bacteriochlorophyll.

**Unit-IV: Enzymes and medicinal Chemistry**

Enzymes and co-enzymes, Structure and function of carboxypeptidase A, Carbonic anhydrase, Xanthine oxidase, Phosphatase, Vitamin B-12, Nitrogen fixation, Biochemical basis of essential metal deficient diseases and their therapies (Iron, Zinc, Copper and Manganese). Chelate therapy, Anticancer drugs-cisplatin.

**Books Recommended:**

- Inorganic Chemistry – Puri, Sharma and Kalia. Milestone publishers, 32<sup>nd</sup> Edn.; 2014
- Inorganic Chemistry, J. E. Huhey, Harpes & Row. 4<sup>th</sup> Edn.; 2008.
- Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
- Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.
- Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
- Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
- The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarendon; 1991
- A Text book of Medicinal aspects of Bioinorganic Chemistry; Das; CBS; 1990.
- Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
- Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976
- Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
- The Inorganic Chemistry of Biological processes; Hughes ; Wiley; 2<sup>nd</sup> Edn.; 1973.

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Discipline Centric**  
**Course Title: Conducting Polymers**  
**Course Code: PCH-DCE-206**

Credits = 3

M.M. = 100 (70+30)

**Unit-I: Basic Concepts**

Basics of conducting polymers, Historical background. Classification of electrochemically active polymers, Redox polymers, Electronically conducting polymers (Intrinsically Conducting Polymers—ICPs), Electronically conducting polymers with built-in or pendant redox functionalities, Copolymers, Composite materials, Applications of conducting polymers.

**Unit-II: Synthesis**

Electrolytic conduction, Electrodes and mechanism; Electrochemical-synthesis of derivatives of poly-pyrrole, Polythiophene, Polyazulene, Polycarbazole, insert inorganic examples.

**Unit-III: Semiconducting and Metallic Polymers**

Introduction and structural basis for semiconducting, metallic polymers and organic meta-polymers- synthetic routes, isomers and electronic structure of polyacetylene, Poly-*p*-phenylene, Polypyrrole, Polythiophene, insert metallic examples

**Unit-IV: Doping and Catalysis**

Introduction, Electrochemical doping, Role of reduction and oxidation potential in doping, Polyacetylene as electrode materials.

Introduction to catalysis, Catalytic properties of conducting polymers, Catalysis of electron donor-acceptor complexes.

Electrocatalysis by semiconducting polymers.

**Books Recommended:**

- Conducting Polymers; A New Era in Electrochemistry, Gyorgy Inzelt, Springer-Verlag Berlin Heidelberg 2<sup>nd</sup> Edn.; 2012.
- Conductive Electroactive Polymers, Wallace Gordon, Gordon G Wallace, Geoffrey M Spinks, CRC Press, 3<sup>rd</sup> Edn.; 2008
- Conductive Polymers and Plastics, Larry Rupprecht, Elsevier, 1<sup>st</sup> Edn.; 2000.
- Handbook of Conducting Polymers, Terje A. Skotheim, Ronald L. Elsenbaumer, John R. Reynolds, Marcel Dekkar, 2<sup>nd</sup> Edn.; 1997.
- Handbook of Organic Conductive Molecules and Polymers, Four Volume Set, Hari Singh Nalwa (Editor), Wiley, 1997.
- Organic Conductors, Jean-Pierre Farges, Marcel Dekkar, 1994
- New Concepts in Polymer Science, Polymeric Composites, Raymond B Seymour, VSP, 1990.
- Electrically Conductive Organic Polymers for Advanced Applications David B Cotts, Z Reyes, 1987.

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Core course**  
**Course Title: Laboratory course in Organic Chemistry**  
**Course Code: PCH-CC-207**

Credits = 2  
M.M. = 100 (70+30)

**Unit-I: Organic Preparations**

- Preparation of dibenzal acetone from benzaldehyde.
- Preparation of adipic acid by chromic acid oxidation of cyclohexanol.
- Preparation of caprolactum.
- Preparation of phenol formaldehyde resin.
- Preparation of cinnamic acid by perkin reaction.

**Unit-II: Qualitative Analysis.**

- Detection of elements: nitrogen, sulphur and halogens.
- Detection of functional groups: detection of carbohydrates, Unsaturation, Carboxylic acids, Carbonyl compounds, Phenols, Alcohols, Halides, Amines, Amides, Imides, Ureas, Thioureas, Nitrocompounds and hydrocarbons.
- Separation and identification of binary organic compounds using physico-chemical methods.

**Books Recommended:**

- Organic Chemistry Lab Manual N. S. Gnanapragasam and B. Ramamoorthy, S. Visvanathan Printers & Publishers, 2010.
- Comprehensive Practical Organic Chemistry; V. K. Ahluwalia and Renu Aggarwal; University Press; 2000
- Advanced Practical Organic Chemistry; N. K. Vishnoi; Vikas; 2<sup>nd</sup> Edn.; 1999.
- Vogel's Textbook of Practical Organic Chemistry; A. R. Tatchell; ELBS; 5<sup>th</sup> Edn.; 1996.
- Experiments and Techniques in Organic Chemistry; D. Pasto, C. Johnson and M. Miller; Prentice-hall; 1992.
- Microscale and Macroscale Organic Experiments; K. L. Williamson; D. C. Heath and Co. 1989.

**M.Sc. FIRST YEAR**  
**Second Semester**  
**Core Course**  
**Course Title: Laboratory course in Analytical Chemistry**  
**Course Code: PCH-CC-208**

Credits = 2  
M.M. = 100 (70+30)

**Unit-I: pH-metry**

- Determination of strength and pK<sub>a</sub> value of a weak acid by titration with an alkali.
- Titration of a dibasic acid with alkali to find its pK<sub>a</sub> values.

**Unit-II: Ion Exchange**

- Determination of Ion-exchange capacity of resin (cationic and anionic).
- Separation of Zn and Cd by ion-exchangers.

**Unit-III: Chromatography**

- Column chromatographic separation of cis and trans azobenzene, determined spectrophotometrically.
- Separation of amino acids by thin layer and paper chromatography.

**Unit-IV: Spectroscopy**

- Extraction of caffeine from tea leaves, characterization by IR.
- Determination of iron in pharmaceutical samples by visible spectrophotometry.

**Unit-V: Quantitative analysis**

- Determination of iodine value and saponification value of edible oils.
- Determination of copper and zinc in brass.
- Determination of metal ions by flame photometry (sodium, potassium, sodium and potassium in a mixture).

**Books Recommended:**

- Environmental Chemistry, A. K. De, 7<sup>th</sup> Edn.; 2010.
- Practical Pharmaceutical Chemistry, part-2, Beckett, Stenlake, 4<sup>th</sup> Edn.; 2001.
- Analytical Chemistry Theory and Practice, R. M. Verma .CBS Publishers & Distributors, 3<sup>rd</sup> Edn.; 2000.
- Vogel's Quantitative Analysis Mendham, Denny; Pearson Education 6<sup>th</sup> Edn.; 2000
- A textbook of Practical Organic Chemistry, A. I. Vogel, 5<sup>th</sup> Edn.; 1996.
- Standard methods of Chemical Analysis, F. J. Welcher, 6<sup>th</sup> Edn.; 1962.
- Experiments in Chemistry, D. V. Jagirdar, Himalaya publication.