Course No: CHM-101
Title: Inorganic Chemistry.

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Stereochemistry and Bonding in the Compounds of Main Group Elements. (14 hrs)

Valence bond theory- Energy changes taking place during the formation of diatomic molecules; factors affecting the combined wave function. Bent's rule and energetics of hybridization.

Resonance: Conditions, Resonance energy and examples of some inorganic molecules/ions.

Odd electron bonds: Types, properties and molecular orbital treatment.

VSEPR: Recapitulation of assumptions; Shapes of Trigonal bypyramidal, Octahedral and Pentagonal bipyramidal molecules / ions. (PCl_5, VO_3^{-1}, SF_6, $[SiF_6]^{2-}$, $[PbCl_6]^{2-}$ and IF_7).

Limitations of VSEPR theory.

Molecular orbital theory- Salient features, Variation of electron density with internuclear distance.

Relative order of energy levels and molecular orbital diagrams of some heterodiatomic molecules /ions.

Molecular orbital diagram of Polyatomic molecules / ions. Walsh diagrams (Concept only).

Delocalized molecular orbitals:- Butadiene, cyclopentadiene and benzene.

Detections of Hydrogen bond: UV – Vis ; IR and X-ray ; Importance of hydrogen bonding.

Unit-II: Bonding in Coordination Compounds and Metal Clusters: (12 hrs)

Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn -Teller distortion, spectrochemical series and the nephleuxetic effect.

Evidence of covalent bonding in transition metal complexes; Adjusted crystal field theory.

Molecular orbital theory of bonding in octahedral complexes:- composition of ligand group orbitals;molecular orbitals and energy level diagram for sigma bonded ML6; Effect of pi-bonding.

Molecular orbital and energy level diagram for Square-planar and Tetrahedral complexes.

Metal Clusters: Introduction to metal clusters; Dinuclear species ; Metal –metal multiple bonds.

Unit-III: Metal- Ligand Equilibria in Solution (10 hrs)

Stepwise and overall formation constants. Factors affecting stability of complexes with respect to the nature of metal ion and ligands. Stability of uncommon oxidation states.

Determination of formation constants by pH- metry and spectrophotometry.

Metal Chelates: Characteristics; Chelate effect and the factors affecting stability of metal chelates.

Applications of metal chelates in chemical analysis and medicine.

Complexes of macrocyclic ligands:- Crown ethers and cryptands.

Unit-IV: pi- Complexes and Iso- Heteropolymetallates of Transition Metals: (14 hours)

Transition Metal Carbonyls: Carbon monoxide as ligand; Synthesis, reactions, structures and bonding of mono- and poly-nuclear carbonyls. Vibrational spectra of metal carbonyls for structural diagnosis.

Prepration, reactions, structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes of transition metals.

Tertiary phosphine as ligand.

ISO - and Heteropolymetallates :-Synthesis, reactions , and structure of polyanions of Vanadium, Molybdenum and Tungsten. Applications of polyacids.

Books Recommended:

1. *Advanced Inorganic Chemistry, 5th ed. / 6th ed., F.A. Cotton , G. Wilkinson ; Wiley 1998/1999*
2. *Inorganic Chemistry, 4th ed. J. E. Huheey, E. A. Keiter….. Harper Collins, 1993.*
3. *Inorganic Chemistry- G. Wulfsberg ; Viva ; 2002*
4. *Chemistry of the Elements 2nd ed. - N. N. Greenwood, A. Earnshaw (Butterworth, 1997)*
5. *Inorganic Chemistry, 3rd ed. - D. F. Shriver, P. W. Atkins ; Oxford, 1999.*
6. *Inorganic Chemistry – K.F. Purcell, J.C Kotz ;Saunders, 1977.*
7. *Coordination Chemistry - D. Banerjea ; Tata McGraw Hill, 1993.*

Course No: CHM-102
Title: Organic Chemistry.

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Delocalized Chemical bonding (12 hrs)

Overview: Inductive effect. Conjugation, Cross conjugation, Hyperconjugation–Isovalent and sacrificial hyperconjugations, Acids / Bases, Nucleophiles and Electrophiles. Resonance, Rules of resonance, Steric inhibition of resonance.

Aromaticity: Huckel rule and concept of aromaticity, Molecular orbital diagram of annulenes, Frost diagram. Relation between NMR and aromaticity.

Annulenes: Systems with electron numbers other than six (2,4,8,10 and more than ten π-electron systems), Aromaticity of hetero annulenes. Aromaticity in fused ring systems. Aromaticity of ferrocene and azulene. Anti and Homoaromaticity

Tautomerism: Different types including valence tautomerism.

Unit -II : Reactive Intermediates and Reaction Mechanism (12 hrs)

Reactive Intermediates: Generation, Structure, fate and stability of carbocations, (Classical and non- classical) carbanions, free radicals, carbenes, nitrenes and radical ions

Reaction Mechanism: Reaction Mechanism & Types of reactions. Determining reaction mechanism: Structure of product, Transition state & intermediate (Hammond postulate). Catalysis including acid and base catalysis, Specific acid and base catalysis. Fate of individual atoms (Isotope Labeling). Stereochemical course of reaction. Thermodynamic and kinetic evidences. Correlation of structure – reactivity. The Hammet relationship.

Unit-III : Aliphatic Nucleophilic Substitutions : (13 hrs)

Mechanism and stereochemical implications of S_N2, S_N1, S_Ni and Neighbouring Group Participation (by π and σ-bonds) reactions. Comparison of S_N1 and S_N2 reactions.Effect of substrate structure, attacking nucleophile, leaving group and solvent on the rates of S_N1 and S_N2 reactions. Mixed S_N1 and S_N2 reactions. Nucleophilic substitution at allylic, benzylic, aliphatic trigonal and vinylic carbons. Nucleophilic substitution in alcohols, Mitsunobu reactions.Substitutions on other elements. Functional group transformation using S_N2 reactions in organic synthesis. Nucleophilic substitutions in biological systems

Elimination reactions: Factors affecting elimination reactions, Mechanism of E1, E2, E1cB and E2C reactions. Competition between substitution and elimination reactions. Stereochemistry and

regioselectivity of E2 eliminations, Elimination in cyclic systems and vinyl halides. Mechanism and orientation in pyrolytic eliminations, Shapiro reaction.

Aliphatic Electrophilic Substitutions

General mechanism of S_E1, S_E2 and S_Ei reactions. Mechanisms of reactions involving migration of double bond. Effect of substrate, leaving group and solvent on reactivity. Stork-enamine reaction.

Unit – IV Stereochemistry: (13 hrs)

Molecular symmetry and Chirality , Chirality due to chiral carbon in other quadrivalent chiral atoms. Chirality in compounds with tervalent chiral atoms. Charality in suitably substituted adamantanes. Charlity due to restricted rotation (leading to perpendicular dissymmetric planes), biphenyls and allenes. Chirality due to helical shape. Chirality / optical activity caused by restricted rotation of other types.

Creating a chiral Centre , molecules with more than one chiral centre, Asymmetric synthesis. Enantiotopic diasteroic topic groups and faces.

Conformational analysis of cycloalkanes, with more than one substituents and decalines. Effect of conformation and reactivity : SN^1 reaction and epoxidation reactions.

Conformation and reactivity of cyclohexene and cyclohexanone. Conformation of sugars , steric strain due to unavoidable crowding.

Books Recommended:

1. *Advanced Organic Chemistry Reactions, Mechanism and Structure, 5th Ed.-Jerry March. (Wiley, 1999).*
2. *Advanced Organic Chemistry 4th Ed. - F. A. Carey and R. J. Sundberg. (Plenum, 2001).*
3. *A Guide Book to Mechanism in Organic Chemistry 6th Ed.- Peter Sykes. (Longman, 1996).*
4. *Structure and Mechanism in Organic Chemistry 2nd Ed. - C. K. Ingold. (CBS, 1994).*
5. *Modern Organic Reactions 2nd Ed. - H.O. House (Benjamin, 1972)*
6. *Principles of Organic Synthesis 2nd Ed. - R.O.C. Norman (Chapmann Hall, 1978)*
7. *Reaction Mechanism in Organic Chemistry 3rd Ed. - S.M. Mukherjee and S.P. Singh. (Macmillan, 1998).*
8. *Stereochemistry of Organic Compounds 2nd Ed.- D. Nasipuri. (New Age Inter., 1994)*
9. *Stereochemistry of Carbon Compounds - E.L.Eliel. (TMH, 1995)*
10. *Stereochemistry of Organic Compounds 3rd Ed. - P.S. Kalsi. (New Age Inter., 1995).*
11. *Organic Chemistry - J. Hornback. (Brooks/Cole, 1998)*
12. *Fundamentals of Organic Chemistry , 5th ed.- Solomons. (Wiley, 1992)*
13. *Organic Chemistry, 5th Ed.- John McMurry. (Brooks/Cole, 2000).*

Course No: CHM- 103
Title: Physical Chemistry

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit-I: Quantum Chemistry (12 hrs)

Exact quantum mechanical results:

Time-independent and time-dependent Schrodinger equation. Postulates of quantum mechanics. Operator concept, quantum mechanical operators in Cartesian and Spherical polar co-ordinate systems, some properties of quantum mechanical operators. Review of particle in a box problem. The solution of problems of harmonic oscillator & the rigid rotator. Tunneling effect.

Unit- II: Statistical Thermodynamics (12 hrs)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. (3 hrs)

Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einestein and Fermi-Dirac laws and their comparison with Boltzmann distribution law. (3 hrs)

Partition function & its significance, translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions , application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions with application to isomerization and atomization reactions.. (6 hrs)

Unit-III: Chemical kinetics –I (12 hrs)

Kinetic analysis of experimental data: Estimation of order and rate constant from concentration-time data (Differential rate method and integral rate method). (2 hrs)

Fast reactions: General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis. (3hrs)

Theories of Chemical Reactions: Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory (3 hrs)

Theories of unimolecular reactions (Lindman, Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces. (4 hrs)

Unit-IV: Chemical kinetics –II **(14 hrs)**

Surface Reactions: Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langnuir- Riedel mechanism], classical & statistical treatments. (4hrs)

Reactions in Liquid solutions: Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, Hammett equation, Taft equation. (5 hrs)

Catalysis: Introduction to catalysis, mechanism of catalysis, use of solvents as catalysts, Enzyme catalysis; Michaelis–Menten Equation, Inhibition of Enzymes, Effects of pH, Temperature Effects. (5hrs)

Books Recommended:

1. *Physical Chemistry - P. W. Atkins, ELBS , Oxford, 1997.*
2. *Physical Chemistry- A Molecular Approach - D. A. McQuarie & J. D. Simon, University Science Books, 1997.*
3. *Introduction to Quantum chemistry - A. K. Chandra, TataMcGraw Hill, 1997.*
4. *Quantum Chemistry - Ira. N. Levine, Prentice Hall, 2000.*
5. *Quantum Chemistry, Prasad, New Age Publishers, 2000.*
6. *An Introduction to Statistical Thermodynamics, Robert P. H. Gasser and W. Graham Richards, World Scientific Publishing Co. 1995*
7. *Statistical Thermodynamics, M.C.Gupta, New Age International, 1993.*
8. *Statistical Mechanics, Agarwal, Eisner, Wiley, 1991.*
9. *Introduction to Statistical Thermodynamics, Chandler, OUP, 1987.*
10. *An introduction to Statistical Thermodynamics, Hill, Addison-wesley, 1987.*
11. *Chemical Kinetics, K. J. Laidler, Mcgraw-Hill, 1987.*
12. *Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989*
13. *Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001*

Course No: CHM-104.
Title: Symmetry and Spectroscopy

Max. Marks: 100 ***Min. Qualifying Marks:*** *40%*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*
Total Duration: *(50 hrs.)*

Unit I: Symmetry -I **(12 hrs)**

Symmetry elements and operations; combination of symmetry operations. Groups, subgroups, classes and group multiplication tables. Symmetry point groups Schoenflies notations of point groups; identification of point groups. Systematic procedure for assignment of point groups to molecules; Symmetry classes and their geometrical significance.

Unit II: Symmetry -II **(12 hrs)**

Matrices and their combinations, block factored matrices; matrix representation of symmetry operation and point groups. Reducible and irreducible representation, character of a representation, properties of irreducible representations, Mulliken Symbols for IRS. Character table, construction of character tables for C2v, C3v and C4v point groups.

Applications of symmetry: Molecular chirality, Polarity, Fluxionality, and IR and Raman spectroscopy.

Unit III: Electronic Spectroscopy **(14 hrs)**

Interaction of light with matter, transition probability, transition moment integral, derivation of selection rules.

Intensity of spectral lines; Einstein's treatment of absorption and emission processes. Oscillator strength.

Natural spectral line width, broadening of spectral lines -Doppler and Collision effects,

Electronic Spectroscopy

Vibronic transitions. Intensity of spectra—the Franck-Condon principle.

Electronic spectra of organic molecules; chromophores , auxochrome, spectral shifts Different types of electronic transitions; nomenclature, symmetry labels of electronic states--spectra of formaldehyde. Effects of solvent, electron withdrawing and electron donating groups, conjugation and extended conjugation on the position of spectral bands.

Photoelectron Spectroscopy

Basic principles- photoionization process; ionization energies; Koopman's theorem. Photoelectron spectra of simple molecules (N_2, O_2), ESCA - Application.

Unit IV: Infrared and Raman Spectroscopy (12 hrs)

Infrared Spectroscopy

Linear harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration-rotation spectra of diatomic molecules; P, Q and R branches;

Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Factors influencing the band positions and intensities. Group frequencies and finger print region.

Raman Spectroscopy

Classical and Quantum theories of Raman scattering, Molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications.

Books Recommended:

1. *Physical Methods for Chemists , 2nd edn. R.S.Drago (Saunders, 1992)*
2. *Fundamentals of Molecular Spectrsocopy, 4th edn- C.N.Banwell, E.M.Mc Cash (Tata McGrawHill, 1994)*
3. *Modern Spectroscopy- J.M.Hollas (Wiley, 1987)*
4. *Basic Principles of Spectroscopy- R.Chang (McGraw Hill, 1971)*
5. *Structural Methods in Inorganic Chemistry, 2nd edn. E.A.V.Ebsworth, D.W.H.Rankin, S.Cradock (Blackwell, 1991)*
6. *Chemical Applications of Group Theory, 2nd edn.-F.A.Cotton (Wiley Eastern, 1994)*
7. *Molecular Symmetry and Group Theory- L.Carter (Wiley 1998)*
8. *Symmetry and Spectroscopy of Molecules- K.Veera Reddy (New Age, 1998).*

Course No: CHM- 105(a)
Title: Mathematics for Chemists

Max. Marks: 50 ***Min. Qualifying Marks:*** *40%*
External Exam: *40 Marks.* ***Internal Assessment****: 10 Marks*
Total Duration: *(25 hrs.)*

Unit-I: **(6 hrs)**

a) Permutations and Probability (3 hrs)

Permutations and combinations. Probability and probability theorems**.** Average, root mean square and most probable errors (examples from kinetic theory of gases)

b) Vectors (3 hrs)

Vectors, dot, cross and triple product. Gradient, divergence and curl of a vector, Determinants, basic concepts, types and properties.

Unit-II: Determinants and Matrix Algebra **(6 hrs)**

Determinants, basic concepts, types and properties

Matrices, addition and multiplication of matrices, inverse, adjoint and tranpose of matrices, special matrices (symmetric, skew-symmetric, hermitian, skew- hermitian, unit, diagonal, unitary matrices.)

Matrix equations: Homogeneous and non-homogeneous linear equations and conditions for their solutions. Eigen-value problem

Unit-III: Calculus (Differentiation and Integration) **(7 hrs)**

Rules for differentiation, applications of differential calculus including maxima & minima finding (Examples: Maximally populated rotational levels, Bohr's radius, most probable velocity from Maxwell distribution), exact and inexact differentials & applications to thermodynamic properties.

Partial differentiation

Integration, basic rules for integration, integration by parts, partial fractions and substitution. Applications of integral calculus.

Co-ordinate transformations (Cartesian to spherical polar co-ordinates)

Unit-IV: Elementary Differential Equations **(6 hrs)**

Variables-separable and exact first order differential equations, homogeneous, exact and linear equation. Solutions of differential equation by power series method, Fourier series, second order differential equations and their solutions. (Applications to chemical kinetics and quantum chemistry.)

Books Recommended:

1. *The Chemistry Mathematics Book, E. Steiner, Oxford.*
2. *Mathematics for Chemistry- G. Doggett & B.T. Sutcliffe, Longmann 1995*
3. *Mathematical Methods for Scientists and Engineers, D. A. McQuarie, University Science Books, 2003.*
4. *Chemical Mathematics D. M. Hirst, Longman.*
5. *Basic Mathematics for Chemists, Tebbutt, Wiley.*
6. *Mathematics for Chemists - C. L. Perrin, Wiley, 1970.*
7. *Mathematical Techniques in Chemistry - J. B. Dence, Wiley, 1975.*
8. *Mathematical Method in Physical Science, M.L. Boas, John Wiley and Sons, 2nd*

Course No: CHM-105(b)
Title: Biology for Chemists

Max. Marks: 50 ***Min. Qualifying Marks:*** *40%*
External Exam: *40 Marks.* ***Internal Assessment****: 10 Marks*
Total Duration: *(25 hrs.)*

Unit I : Cell Structure and Function (5 hrs)

1. Structure of prokaryotic and Eukaryotic cell;
2. Intracellular organelles and their function**;**
3. Composition of plant and Animal cell;
4. Bio-Membranes: Fluid Mosaic Model structure and
5. Function of different components -Micelles bilayers,
6. Liposomes.

Unit II: Bio molecules and their role in living systems (5 hrs)

1.	Monosaccharides:	Overview of stucture & functions
2.	Disaccharides	Overview of stucture & functions
3.		Polysaccharides Cellulose; Chitin details of stucture & functions
4.	Macromolecules	Starch; Glycogen, Proteins (Glycoproteins, lipoproteins
		Lipids; polysaccharides stucture & functions.)

Unit III: Life Molecules and Metabolic Processes (5hrs)

1. Properties of carbon, chemical evolution and Evolution of Living systems;
2. General idea of various metabolic processes of living Organism (Catabolism/anabolism)
3. Elementary idea of different metabolic cycles (Kreb's cycle, Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenessis, pentose phosphate pathway)
4. Biosynthesis of Amino Acids and their degradation
   Tryptophan Releasing Hormone

Unit IV: Chemical Basis of Heredity (10 hrs)

1. Nuclic Acids and their Role in heredity, DNA Replication, Transcription and translation, General idea of Genetic code.
2. Structure of purine and pyrimidine bases, Overview of DNA and RNA, Double helix model of DNA, Mono and trinucleoside- A general idea

Books Recommended:

1. Biochemistry and Physiology 4th edn by Salisbvry and Ross.
2. Principles of Biochemistry, A.L.Lehninger, Worth Publishers
3. Biochemistry, L.Stryer, W.H.Freeman.
4. Biochemistry, J.David Rawn, Neil Patterson.
5. Biochemistry, Voet and Voet, John Wiley.
6. Outlines of Biochemistry. E.E.Conn and P.K.Stumpf, John Wiley

Course No. CHM-106L
Title: Laboratory Course in Inorganic Chemistry

Max. Marks: 150 ***Min. Qualifying Marks:*** *40%*
External Exam: *120 Marks.* ***Internal Assessment****: 30 Marks*
Total Duration: *(150 hrs.)*

1. **Qualitative Analyses:**

   Identification of cations including those of less common elements using Semi-micro technique.

2. **Quantitative Analyses:**

   Estimation of Cations in two- cation systems using gravimetric and volumetric (EDTA or Redox) methods.

3. **Preparation of Coordination Compounds of transition metals.**

4. **Paper Chromatography:**

   Separation and identification of Cations from mixtures containing two or three cations.

Books Recommended*:*

1. *Vogel's Qualitative Inorganic Analysis; 6th edn; Svehla (Longman, 1994)*
2. *The physical Chemistry of Inorganic Qualitative analysis; Kuriacose, Rajaram (Tata MGH, 1972).*
3. *Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; (ELBS, 1989).*
4. *Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).*
5. *Chromatographic Methods; 3rd ed; Stock & Rice (Chapman & Hall, 1980).*
6. *Analytical Chemistry; 5th ed; D. Christian (Wiley)*