

University of Kashmir

Department of Chemistry

DST Assisted Under FIST

Semester-wise Syllabi for M.Sc. Programme in Chemistry

(M.Sc. Ist Semester)

Course No: CHM-101
Title: Inorganic Chemistry

Max. Marks- 100

(50 hrs)

Unit I: Stereochemistry and Bonding in Main Group Compounds (10 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.

Molecular orbital theory- Variation of electron density with internuclear distance; overlap integral. . Molecular orbitals and molecular structure - Walsh diagrams (tri- and tetra- atomic molecules).

Delocalized molecular orbitals:- Butadiene, cyclopentadiene and benzene.

VSEPR: Shape of molecules and ions; limitations

Hydrogen bond: Detection, theories, effect on properties and π - hydrogen bonding.

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

Unit II:

A: 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 and detection of chelates; the 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.

B: Metal-Ligand Bonding: (10 hrs)

Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn -Teller distortion, spectrochemical series and the nephelauxetic 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 ML_6 ; effect of pi-bonding.

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

Unit-III: pi- Complexes of Transition Metals : (10 hrs)

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

Preparation, reactions, structure, bonding of transition metal Nitrosyls, and Dinitrogen and Dioxygen complexes of transition metals.

Tertiary phosphine as ligand.

Unit IV: Organometallic Compounds: (10hrs)

Definition, nomenclature and classification of organometallic compounds. Effective atomic number (18-electron) rule. Stability of organometallic compounds towards heat, oxidation and hydrolysis.

Preparation, properties, structure and bonding, and applications of alkyls and aryls of Li, B, Al and Sn.

Synthesis, structure and bonding of metal-alkene complexes with special reference to Zeise's salt. Homogeneous hydrogenation.

Books Recommended:

1. Advanced Inorganic Chemistry, 6th ed. /5th ed. F.A. Cotton , G. Wilkinson (Wiley 1999/1988)
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. Principles of Organometallic Chemistry, 2nd ed. P. Powell (Chapman & Hall, 1988)
7. Organometallic Chemistry - R. C. Mehrotra, A. Singh (Wiley Eastern, 1991)
8. Coordination Chemistry - D. Banerjee (Tata McGraw Hill, 1993)

Course No: CHM-102
Title: Organic Chemistry.

Max. Marks- 100 **(50 hrs)**

Unit-I: Delocalised Chemical bonding **(13 hrs)**

Conjugation, Cross conjugation, rules of resonance, steric inhibition of resonance.
Aromaticity: Huckel rule and concept of aromaticity, Molecular orbital description of aromaticity and antiaromaticity. Relation between NMR and aromaticity. Annulenes (Two to more than ten π -electron systems), Aromaticity of hetero annulenes and fullerenes (C-60). Homoaromaticity.
Hyperconjugation: Explanation of hyperconjugative effect, isovalent and sacrificial hyperconjugations
Tautomerism: Different types including valence tautomerism.
Reactive Intermediates: Generation, Structure, fate and stability of carbocations, (Classical and non- classical) carbanions, free radicals, carbenes, nitrenes and radical ions.

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

Elements of symmetry, Chirality due to chiral centre, molecules with more than one chiral centre, threo and erythro isomers optical activity in the absence of chiral carbon (biphenyls, allenes and spirans). Chirality due to helical shape. Enantiotopic and diastereotopic atoms, groups and faces.

Asymmetric synthesis, Stereospecific reactions (Diels Alder reaction, anti addition of halogens, enzyme catalysed reactions and Rhodium complex reaction). Stereoselective synthesis of ephedrine and epiandrosterone and pheromone.
Conformational analysis of cycloalkanes and decalines. Effect of conformation and reactivity in acyclic and cycloalkanes. Conformation of sugars, steric strain due to unavoidable crowding.

Unit -III: **(13 hrs)**

A: Reaction Mechanism/ Structure and reactivity

Types of mechanisms. Types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates. Methods of determining reaction mechanism, isotope effects. **Effect of structure on reactivity:** Resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

B: 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 :

(12 hrs)

A: Aliphatic Nucleophilic Substitution

Mechanisms and stereochemical implications of S_N2 , S_N1 , S_{Ni} and neighbouring group participation (by π and σ -bonds) 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, aliphatic trigonal and vinylic carbon.

B: Elimination reactions:

Discussion of E1, E2, E1cB and E2C mechanisms. Effect of substrate structure base and the leaving group on reactivity. Competition between substitution and elimination reactions. Stereochemistry and orientation of E2 elimination. Mechanism and orientation in pyrolytic eliminations, Shapiro reaction.

Books Recommended:

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, 4th 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.Elial. (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

(50 hrs)

Unit-I: Quantum Chemistry-I

(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: Quantum Chemistry-II

(12 hrs)

Born-Oppenheimer approximation. Solution of the Hydrogen-like atom problem- radial and angular wave functions.5

Angular momentum and electronic structure of atom

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Wave functions of poly-electron atoms, Slater determinant. Atomic term symbols, term separation of p^n and d^n configurations, spin-orbit coupling, Zeeman splitting. ...7 hrs

Unit-III: Thermodynamics of electrolyte solutions

(12 hrs)

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 co-efficients. 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-IV: Chemical kinetics –I**(14 hrs)**

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

Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory ...3 hrs

Dynamics of unimolecular reactions (Lindman-Hinshelwood , RRK and RRKM theories), Introduction to potential energy surfaces. ...2 hrs

Surface Reactions: Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langmuir- Riedel mechanism], classical & statistical treatments. ...2hrs

Ionic Reactions: Single & double sphere models of ionic reactions. Diffusion controlled reactions (partial & full microscopic diffusion control) ...2 hrs

Chain Reactions: Thermal Hydrogen-Bromine reaction, explosive reactions, oscillatory reactions (BZ reaction) ...2hrs

Books Recommended:

1. Physical Chemistry - P. W. Atkins, ELBS , Oxford, 1997.
2. Physical Chemistry- A Molecular Approach - D. A. McQuarrie & 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. Chemical Kinetics, K. J. Laidler, McGraw-Hill, 1987.
7. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
8. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
9. Modern Electrochemistry Vol-I and Vol-II, J.O.M. Bockris and A.K.N. Reddy, Plenum, 1998.
10. Electrochemical methods, Fundamentals and Methods, A.J. Bard, L.R. Faulkner, Wiley, 1980.
11. Chemical Thermodynamics, Rastogi & Mishra, Vikas Publishing, 1996.
12. Chemical Thermodynamics, P. A. Rock, Uni. Sci. Books, 1983.

Course NO: CHM-104.

Title: Group Theory and Spectroscopy

Max. Marks- 100

(50 hrs)

Unit I: Symmetry and Group Theory-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 and Group Theory-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 C_{2v} , C_{3v} and C_{4v} point groups.

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

Unit III: Electronic Spectroscopy

(12 hrs)

Uncertainty relation and natural line width, spectral line broadening-Doppler and Collision effects, transition probability, transition moment, selection rules, intensity of spectral lines.

Molecular Spectroscopy

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

Electronic spectra of polyatomic molecules (Conjugation, extended conjugation, and effect of steric hindrance).

Electronic spectra of transition metal complexes (d-d, intraligand, and charge transfer transitions), donor-acceptor complexes of organic molecules.

....7hrs

Photoelectron Spectroscopy

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

Auger electron spectroscopy- basic idea.

Unit IV: Microwave and Infrared spectroscopy

(14 hrs)

Moment of inertia, classification of molecules according to their moment of inertia. The rigid diatomic molecule – Classical rotation, quantization of rotational angular momentum, allowed rotational energies. Pure rotation spectra of rigid diatomic molecule; selection rules, intensities of spectral lines, the non-rigid rotor, effect of isotopic substitution. Applications.

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 diagram. Vibration-rotation spectra of diatomic molecules; P, Q and R branches;

Vibrations of polyatomic molecules: Fundamental vibrations, selection rules; overtones, combination and difference bands, hot bands. Group frequencies and finger print region. Factors influencing the band positions and intensities. Far infrared region, Metal-Ligand vibrations.

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 Spectroscopy, 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

(25 hrs)

Unit-I:

a) Permutations and probability: (3hrs)

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, vector calculus.

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

Determinants, basic concepts, types and properties
Matrices, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew-symmetric, hermitian, skew- hermitian, unit, diagonal, unitary.)
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 Engineering, 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 Methods for Physical Sciences, M. L. Boas, Wiley.

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

Max. Marks- 50

(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)

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

Lipids; polysaccharides structure & 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, Gluconeogenesis, pentose phosphate pathway)
4. Biosynthesis of Amino Acids and their degradation
Tryptophan Releasing Hormone

Unit IV: Chemical Basis of Heredity

(10 hrs)

1. Nuclie 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 Salisbry 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- 100

(100 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)