Course code: CH103R1
Course title: Inorganic Chemistry-I: Atomic Structure & Chemical Bonding-I
Pre-requisite(s): Intermediate level Chemistry
Co- requisite(s):
Credits: 4 L: 4 T: 0 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. I
Branch: Chemistry
Name of Teacher:

Module- I: Atomic Structure (10 Lectures)

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Module- II: Periodicity of Elements (9 Lectures)

s, *p*, *d*, *f* block elements, the long form of periodic table. Effective nuclear charge, Slater rules, Atomic, Ionic & Covalent radii, Ionization enthalpy, Electron gain enthalpy, Electronegativity scales, Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Module- III: Chemical Bonding I (9 Lectures)

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.
(ii) *Metallic Bond:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.
(iii) *Weak Chemical Forces:* van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Module- IV: Chemical Bonding II (10 Lectures)

Covalent bond: Lewis structure, Valence Bond theory, Hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of homo & hetro, di & triatomic molecules Valence shell electron pair repulsion theory (VSEPR), Covalent character in ionic compounds, Fajan's rules, Ionic character in covalent compounds: Bond moment, dipole moment and electronegativity difference.

Module- V: Oxidation-Reduction (7 Lectures)

Redox equations, Standard Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class.

Text books:

1. Lee, J. D. Concise Inorganic Chemistry ELBS, 1991.
2. Douglas, B. E. and McDaniel, D. H. Concepts & Models of Inorganic Chemistry Oxford, 1970.

Reference books:

1. Atkins, P. W. & Paula, J. Physical Chemistry, 10th Ed., Oxford University Press, 2014.
2. Day, M. C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications, 1962.
3. Rodger, G. E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.

Course code: CH113
Course title: Physical Chemistry-I
Pre-requisite(s): Intermediate Level Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. I
Branch: Chemistry
Name of Teacher:

Module I: Gaseous state: ***Kinetic molecular model of a gas*** ***(10 Lectures)***
Postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, relation between mean free path and coefficient of viscosity, variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Module II: Gaseous state: *Behaviour of real gases* ***(12 Lectures)***
Deviations from ideal gas behaviour, compressibility factor, *Z*, and its variation with pressure for different gases. van der Waals equation of state, its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); virial equation of state, calculation of Boyle temperature from virial form. Continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Module III: Liquid state **(10 Lectures)**
Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

Module IV: Symmetry **(08 Lectures)**
Elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices.

Module V: Solid state **(10 Lectures)**
Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

Text books:
1. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 1, Macmillan Publishers India Ltd, 2004
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 10th Ed., Oxford University Press (2014).
3. Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).

Reference books:
1. Ball, D. W. Physical Chemistry Thomson Press, India (2007).
2. Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
3. Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).

Course code: CH105
Course title: INORGANIC CHEMISTRY- I LAB
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. I
Branch: Chemistry
Name of Teacher:

Syllabus

(A) Titrimetric Analysis
(i) Calibration and use of apparatus
(ii) Preparation of solutions of different Molarity/Normality of titrants
(B) Acid-Base Titrations
(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.
(iii) Estimation of free alkali present in different soaps/detergents
(C) Oxidation-Reduction Titrimetry
(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
(iii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

Reference book:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

Course code: CH106R1
Course title: Physical Chemistry-I Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. I
Branch: Chemistry
Name of Teacher:

Syllabus

1. **Surface tension measurements.**
a. Determine the surface tension by (i) drop number (ii) drop weight method.
b. Study the variation of surface tension of detergent solutions with concentration.
2. **Viscosity measurement using Ostwald's viscometer**.
a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
b. Study the variation of viscosity of sucrose solution with the concentration of solute.
3. Indexing of a given powder diffraction pattern of a cubic crystalline system.
Any other experiment carried out in the class.

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course code: CH114
Course title: Physical Chemistry-II
Pre-requisite(s): Intermediate level Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. II
Branch: Chemistry
Name of Teacher:

Module I: Basic Thermodynamics I (15 lectures)

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, q, work, w, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, calculations of q, w, U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Module II: Basic Thermodynamics II (10 lectures)

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Module III: Basic Thermodynamics III (15 lectures)

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Module IV: Systems of Variable Composition (8 lectures)

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Module IV: Chemical Equilibrium (12 lectures)

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p, K_c and K_x. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Text books:

1. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 2, Mcmillan Publishers India Ltd,2004.
2. Peter, A. & Paula, J. de. Physical Chemistry 10th Ed., Oxford University Press (2014).
3. Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).

Reference books:

1. Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
2. McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi (2004).
3. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
4. Levine, I. N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
5. Metz, C. R. 2000 solved problems in chemistry, Schaum Series (2006).

Course code: CH108R1
Course title: Organic Chemistry-I
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. II
Branch: Chemistry
Name of Teacher:

Module-1: Bonding and physical properties. (10 lectures)

(i) *Valence Bond Theory:* Hybridisation, resonance, hyperconjugation, formal charges and DBE; orbital pictures of bonding systems. (ii)*Electronic displacements:* Inductive effect, field effect, mesomeric effect, resonance energy *(iii) MO theory:* Qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ, σ^*, π, π^*, n – MOs; concept of HOMO, LUMO and SOMO, Frost diagram. (iv) *Physical properties:* BDE and bond energy; bond distances, bond angles; concept of bond angle strain; melting point/boiling point. v) *Concept of organic acids and bases*

Module-2: General treatment of reaction mechanism (10 lectures)

(i) Mechanistic classification: Nature of bond cleavage and bond formation, (elementary idea). *Reactive intermediates:* Carbocations, non-classical cabocations, carbanions, carbon radicals, carbenes. (ii) *Reaction thermodynamics:* Free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change *via* BDE, intermolecular & intramolecular reactions. (iii) *Tautomerism*. (iii) *Reaction kinetics:* Rate constant and free energy of activation; free energy profiles; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect, Hammond's postulate.

Module-3: Stereochemistry I (10 lectures)

(i) *Bonding geometries of carbon compounds and representation of molecules:* Fischer, sawhorse, flying wedge and Newman projection. (ii) *Concept of chirality and symmetry.* (iii) *Relative and absolute configuration.* (iv) *Optical activity of chiral compounds.*

Module-4: Stereochemistry II (10 lectures)

(i)Chirality arising out of stereoaxis: allenes, spiro compounds. (ii) Concept of Pro stereoisomerism: Conformation: Conformational nomenclature: eclipsed, staggered, gauche, synandanti; dihedral angle, torsion angle;Klyne-Prelog terminology; P/M descriptors; energy barrier of rotation, concept of torsional and steric strains, dipole-dipole interaction and H-bonding; butane gauche interaction; conformational analysis of ethane, propane, n-butane.

Module 5: Cycloalkanes and Conformational Analysis (5 Lectures)

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams.

Text books:

1. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Reference books:

1. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
2. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
3. McMurry, J. E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

Course code: CH109R1
Course title: Physical Chemistry-II Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2.0 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. II
Branch: Chemistry
Name of Teacher:

Syllabus

Thermochemistry

(a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).

(b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) Calculation of the enthalpy of ionization of ethanoic acid.

(d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.

(f) Determination of enthalpy of hydration of copper sulphate.

(g) Study of the solubility of benzoic acid in water and determination of ΔH.

Any other experiment carried out in the class.

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Athawale, V. D. & Mathur, P. Experimental Physical Chemistry New Age International: New Delhi (2001).

Course code: CH110R1
Course title: Organic Chemistry-I Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. II
Branch: Chemistry
Name of Teacher:

Syllabus

Experiments: Qualitative analysis of single solid organic compounds

1. Detection of special elements (N, S, Cl, Br) by Lassaigne's test
2. Solubility and classification (solvents: H_2O, 5% HCl, 5% NaOH and 5% $NaHCO_3$)
3. Detection of the following functional groups by systematic chemical tests: aromatic amino ($-NH_2$), aromatic nitro ($-NO_2$), amido ($-CONH_2$, including imide), phenolic –OH, acid groups, carbonyl (distinguish between -CHO and >C=O); only one test for each functional group is to be reported.
4. Melting point of the given compound.
5. Preparation, purification and melting point determination of a crystalline derivative of the given compound.
6. Identification of the compound through literature survey.

Reference Books:

1. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry, Pearson Education (2009).
2. Furniss, B. S.; Hannaford, A. J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).

Course code: CH201R1
Course title: Inorganic Chemistry-II
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry
Name of Teacher:

Module I: General Principles of Metallurgy (9 Lectures)
Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining. Metallurgy of selected metals.

Module II:Acids and Bases (9 Lectures)
Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle, Non aqueous solvents

Module III: Chemistry of *s* and *p* Block Elements-I (9 Lectures)
Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements. Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses: Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur,

Module IV: Chemistry of *s* and *p* Block Elements-II (9 Lectures)
Interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens. Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2, XeF_4 and XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

Module V: Inorganic Polymers (9 Lectures)
Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates. Inorganic & Organic hybrid polymers.

Text books:
1. Lee, J. D. Concise Inorganic Chemistry, ELBS, 1991.
2. Douglas, B.E; Mac Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
3. Greenwood, N. N. & Earnshaw, E. A. Chemistry of the Elements, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.

Reference books:
1. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
2. Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010.19
3. Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).

Course code: CH215
Course title: Physical Chemistry-III
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry

Module I: Quantum Chemistry I (13 lectures)

Black body radiation, Planck's quantum theory, wave – particle duality, uncertainty principle, Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (1D, 2D and 3D rigorous treatment). Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Module II: Quantum Chemistry II (08 lectures)

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Module III: Chemical Bonding (8 lectures)

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

Module IV: Molecular Spectroscopy I (13 lectures)

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Module V: Molecular Spectroscopy II (08 lectures)

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Text books:

1. Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
2. Atkins, P.W. and Friedman, R.S. Molecular Quantum Mechanics, 4th edition, Oxford University Press. Oxford, 2005.
3. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 4, Macmillan Publishers India Ltd, 2004
4. Prasad, R.K. Quantum Chemistry, 3rd edition, New Age International, 2006.
5. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).

Reference books:

1. House, J. E. Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA (2004).
2. Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).
3. Kakkar, R. Atomic & Molecular Spectroscopy: Concepts & Applications, Cambridge University Press (2015).

Course code: CH216
Course title: Organic Chemistry-II
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry

Module-1: Chemistry of alkenes (10 lectures)

Addition to C=C: Mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation,*syn* and *anti*-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; Simmons-Smith cyclopropanation reaction; electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; mechanism of allylic and benzylic bromination in competition with brominations across C=C; use of NBS; Birch reduction of benzenoid aromatics.

Module-2: Chemistry of alkynes (5 lectures)

Addition to C≡C (in comparison to C=C): Mechanism, reactivity, regioselectivity (Markownikoff and anti-Markownikoff addition) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity; interconversion of terminal and non-terminal alkynes.

Module-3: Carbonyl and related compounds (10 lectures)

(i) *Addition to C=O:* Structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig and Corey-Chaykovsky reaction; Rupe rearrangement, oxidations and reductions: Clemmensen, Wolff-Kishner, $LiAlH_4$, $NaBH_4$, MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.(ii) *Nucleophilic addition to α,β-unsaturated carbonyl system:* Michael reaction, Stetter reaction, Robinson annulation.(iii) S*ubstitution at sp^2 carbon (C=O system):* Mechanism: $B_{AC}2$, $A_{AC}2$, $A_{AC}1$, $A_{AL}1$ (inconnection to acid and ester); .

Module-4: Substitution reactions (13 lectures)

Free-radical substitution reaction: Halogentaion of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.

Nucleophilic substitution reactions: Substitution at sp^3 centre[systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides, *a*-halocarbonyls]:mechanisms (with evidence),relative rates& stereochemical features: S_N1, S_N2 (Mitsunobu reaction), S_N2', S_N1' (allylic rearrangement) and S_Ni; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP (with hetero atoms and aryl groups); role of crown ethers and phase transfer catalysts.

Module-5: Elimination reactions and aromatic substitution (12 lectures)

(i)*Elimination reactions:* E1, E2, E1cB and Ei (pyrolytic *syn* eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann)and stereoselectivity; comparison between substitution and elimination. (ii) *Electrophilic aromatic substitution:* Mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbonelectrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch,Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmitt); Ipso substitituion.(iii)Nucleophilic aromatic substitution: Addition-elimination mechanism and evidences in favour of it; SN1 mechanism; cine substitution (benzyne mechanism), structure of benzyne.

Text books:

1. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Reference books:

1. Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
2. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

Course code: CH204
Course title: Inorganic Chemistry-II Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M.Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry
Name of Teacher:

Syllabus

(A) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
(ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
(iii) Estimation of available chlorine in bleaching powder iodometrically.

(B) Inorganic preparations

(i) Cuprous Chloride, Cu_2Cl_2
(ii) Preparation of Manganese(III) phosphate, $MnPO_4.H_2O$
(iii) Preparation of Aluminium potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.

Reference Books:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

Course code: CH205R1
Course title: Physical Chemistry-III Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry
Name of Teacher:

Syllabus

UV/Visible spectroscopy

I. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).

II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.

III. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colorimetry

I. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

II. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.

III. Study the kinetics of iodination of propanone in acidic medium.

IV. Determine the amount of iron present in a sample using 1,10-phenathroline.

V. Determine the dissociation constant of an indicator (phenolphthalein).

VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

VII. Analysis of the given vibration-rotation spectrum of HCl

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course code: CH206R1
Course title: Organic Chemistry-II Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P:3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. III
Branch: Chemistry
Name of Teacher:

Syllabus

A. The following reactions **(any eight)** are to be performed, noting the yield of the crude product: (Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield).

1. Nitration of aromatic compounds.
2. Condensation reactions
3. Hydrolysis of amides/imides/esters
4. Acetylation of phenols/aromatic amines
5. Brine mediated benzoylation of amines/amino acids.
6. Side chain oxidation of aromatic compounds
7. Diazo coupling reactions of aromatic amines
8. Bromination of anilides using green approach (Bromate-Bromide method).
9. Redox reaction including solid-phase method.
10. Green 'multi-component-coupling' reaction.
11. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline

B. Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.
C. Melting point of the purified product is to be noted.

Reference Books:

1. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
2. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012).
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

Course code: CH207R1
Course title: Inorganic Chemistry-III
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Module-I: Coordination Chemistry (12 Lectures)
Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, CFSE in weak and strong fields, Octahedral vs. tetrahedral coordination, Jahn-Teller theorem, square planar geometry.
Qualitative aspect of Ligand field and MO Theory. IUPAC nomenclature, Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

Module-II: Transition Elements (10 Lectures)
General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Bsworth diagrams). Difference between the first, second and third transition series. Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy).

Module-III: Lanthanoids and Actinoids (7 Lectures)
Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only).

Module-IV: Bioinorganic Chemistry (9 Lectures)
Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium/K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron.

Module-V: Basic Nuclear Chemistry (7 Lectures)
Systematic of alpha, beta and gamma decays, Alpha decay, energy curve, spectra of alpha particles, Geiger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect.

Text books:
1. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
2. Huheey, J. E., Inorganic Chemistry, Prentice Hall, 1993.
3. Lippard, S. J. & Berg, J. M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
4. Cotton, F. A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999

Reference books:
1. Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
2. Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.

Course code: CH217
Course title: Physical Chemistry-IV
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Module I: Chemical Kinetics (10 lectures)

Order and molecularity, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Arrhenius equation; activation energy. Collision theory, Transition state theory, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

Module II: Catalysis (08 lectures)

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Module III: Electrochemistry (12 lectures)

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules. Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells.

Module IV: Photochemistry (10 lectures)

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. photostationary states, chemiluminescence.

Module V: Surface chemistry (08 lectures)

Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state.

Text books:

1. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 5, Macmillan Publishers India Ltd, 2004
2. Atkins, P. & Paula, J. D. Physical Chemistry 10th Ed., Oxford University Press (2014).
3. Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
4. Rohatgi-Mukherjee, K. K. Fundamentals of Photochemistry, New Age International Pvt. Ltd.; 3rd edition, New Delhi, 2014.

Reference books:

1. Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
2. Zundhal, S. S. Chemistry concepts and applications Cengage India (2011).
3. Ball, D. W. Physical Chemistry Cengage India (2012).
4. Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
5. Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

Course code: CH218
Course title: Organic Chemistry-III
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Module-1: Exploitation of acidity of α-H of C=O (10 lectures)

Exploitation of acidity of α-H of C=O: Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation, SeO2 (Riley) oxidation; condensations (mechanism with evidence): Aldol,Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

Module-2: Organometallics. (09 lectures)

Grignard reagent, Organolithium, Gilman cuprates: Preparation and reactions (mechanism with evidence); addition of Grignard and organolithium to carbonyl compounds; substitution on -COX; directed ortho metalation of arenes using organolithiums, Shapiro reaction, conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behavior of Grignard reagents; comparison of reactivity among Grignard, organolithiums and organocopper reagents; Reformatsky reaction; Blaise reaction; concept of umpolung.

Module-2: Nitrogen compounds (09 lectures)

Nitrogen compounds: (i). *Nitro compounds:* Preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis, Henry reaction and conjugate addition of nitroalkane anion. *(ii). Amines:* Preparation amines; reaction (with mechanism): Eschweiler–Clarke methylation, diazo coupling reaction, formation and reactions of phenylenediamines, diazomethane and diazoacetic ester. *Diazonium salts and their* reactions: Gomberg, Japp-Klingermann. *(iii). Alkylnitrile and isonitrile*: Preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.

Module 3: Rearrangements: **(12 lectures)**

(i). Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzil-benzilic acid rearrangement, Demjanov rearrangement. *(ii). Rearrangement to electron-deficient nitrogen:* rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann. *(iii). Rearrangement to electron-deficient oxygen:* Baeyer-Villiger oxidation, cumene hydroperoxide-phenol rearrangement and Dakin reaction. *(iv). Aromatic rearrangements:* Fries rearrangement and Claisen rearrangement. *(v). Migration from nitrogen to ring carbon*: Hofmann-Martius rearrangement**,** Orton rearrangement and benzidine rearrangement.

Module-5: Spectroscopy I (10 lectures)

(i)UV Spectroscopy: Introduction; types of electronic transitions, end absorption; Bathochromic and Hypsochromic shifts; λmax for the following systems: conjugated diene, α,β-unsaturated aldehydes and ketones(alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of λmax considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.(ii) IR Spectroscopy: Introduction; modes of molecular vibrations (fundamental); characteristic and diagnostic stretching frequencies of C-H, N-H, O-H, C-O, C-N, C-X, C=C (including skeletal vibrations of aromatic compounds), C=O, C=N, N=O, C≡C, C≡N; characteristic/diagnostic application in functional group analysis.

Text books:

1. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Willy & Sons (1976).

Reference books:

1. Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
2. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.

Course code: CH210

Course title: Inorganic Chemistry-III Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Syllabus

Gravimetric Analysis:

i. Estimation of nickel(II) using Dimethylglyoxime (DMG).

ii. Estimation of copper as CuSCN

iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

iv. Estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

Inorganic Preparations:

i. Tetraamminecopper(II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

ii. *Cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate(III)

iii. Tetraamminecarbonatocobalt(III) ion

iv. Potassium tris(oxalate)ferrate(III)

Chromatography of metal ions

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

i. Ni (II) and Co (II)

ii. Fe (III) and Al (III)

Reference Book:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

Course code: CH211R1
Course title: Physical Chemistry-IV Lab
Pre-requisite(s): Intermediate level Chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Syllabus

Kinetics

Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction

2. Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

3. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Conductometry

4. Determination of cell constant

5. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

6. Perform the following conductometric titrations:

i. Strong acid vs. strong base
ii. Weak acid vs. strong base
iii. Mixture of strong acid and weak acid vs. strong base
iv. Strong acid vs. weak base

Potentiometry

7. Perform the following potentiometric titrations:

i. Strong acid vs. strong base
ii. Weak acid vs. strong base
iii. Dibasic acid vs. strong base
iv. Potassium dichromate vs. Mohr's salt

Adsorption

8. Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course code: CH212R1
Course title: Organic Chemistry-III Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. IV
Branch: Chemistry
Name of Teacher:

Syllabus

Identification of the pure compounds.
Solid compounds: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid, salicylic acid, beta-naphthol, lactose and starch.
Liquid Compounds: formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline,dimethylaniline, benzaldehyde, chloroform, nitrobenzene, benzyl alcohol and glycerin.

Reference Books:

1. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry, Pearson Education (2009)
2. Furniss, B. S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
3. Ahluwalia, V. K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
4. Ahluwalia, V. K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

Course code: CH326
Course title: Physical Chemistry-V
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry

Module I: Phase Equilibria I (10 lectures)

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for non-reactive and reactive systems; Clausius-Clapeyron equation and its applications in phase equilibria, phase diagram for one component systems, with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Three component systems, water-chloroform-acetic acid system, triangular plots.

Module II: Phase Equilibria II (10 lectures)

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.

Module III: Solutions and Colligative Properties (08 lectures)

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions. Thermodynamic derivation using chemical potential (i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Module IV: Ionic Equilibria (12 Lectures)

Strong, moderate and weak electrolytes, degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment). Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer action; buffer capacity derivation of Henderson equation and its applications; Solubility and solubility product of sparingly soluble salts–applications. Qualitative treatment of acid–base titration curves. Theory of acid–base indicators; selection of indicators and their limitations. Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Module V: Electrical & Magnetic Properties of Atoms and Molecules (10 lectures)

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mossotti equation, Lorentz-Lorentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement, molecular interpretation.

Text books:

1. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 1, Macmillan Publishers India Ltd, 2004
2. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 2, Macmillan Publishers India Ltd, 2004
3. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 3, Macmillan Publishers India Ltd, 2004
4. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 10th Ed., Oxford University Press (2014).
5. Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).

Reference books:

1. Ball, D. W. Physical Chemistry Thomson Press, India (2007).
2. Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
3. Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).

Course code: CH327
Course title: Organic Chemistry-IV
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Module-1: Organic spectroscopy II **(10 lectures)**

(i) NMR Spectroscopy: Introduction;mbasic principles of Proton Magnetic Resonance; choice of solvent and internal standard; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect;nsignificance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of *first-order*multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR ; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds; rapid proton exchange. (ii) *Mass Spectroscopy:* Basic principle, McLafferty rearrangement metastable peak, General fragmentation mode, isotopic pattern for one halogen atom.

Module 2*:* **(05 lectures)**

Applications: IR, UV, NMR and Mass spectroscopy for identification of organic molecules.

Module-3: Carbohydrates **(12 lectures)**

(i)Monosaccharides: Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms): Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine-water oxidation, HNO_3 oxidation, selective oxidation of terminal $–CH_2OH$ of aldoses, reduction to alditols, (ii) Lobry de Bruyn-van Ekenstein rearrangement; stepping–up (Kiliani-Fischer method) and stepping–down (Ruff's &Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene and benzylidene protections; ring size determination; Fischer's proof of configuration of (+)-glucose. (iii) *Disaccharides:* Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor, structure of sucrose, inversion of cane sugar.

Module-4: Pericyclic reactions **(13 lectures)**

(I) Mechanism, stereochemistry, regioselectivity in case of (ii)Electrocyclic reactions: FMO approach involving 4π- and 6π-electrons (thermal and photochemical) and corresponding cycloreversion reactions. (iii) *Cycloaddition reactions:*FMOapproach, Diels-Alder reaction, photochemical [2+2] cycloadditions.(iv) *Sigmatropic reactions:* FMO approach,sigmatropic shifts and their order; [1,3] and [1,5] H shifts and [3,3] shifts with reference to Claisen and Cope rearrangements.

Module-5: Heterocycles **(10 lectures)**

Heterocyclic compounds: 5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole,thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist-Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzschsynthesis;benzo-fused 5-and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approachand mechanistic details): indole: Fischer,quinoline: Skraup, isoquinoline: Bischler-Napieralski synthesis.

Text books:

1. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Reference books:

1. Berg, J. M., Tymoczko, J. L. & Stryer, L. Biochemistry. 6th Ed. W.H. Freeman and Co. (2006).
2. Nelson, D. L., Cox, M. M. & Lehninger, A.L. Principles of Biochemistry. IV Edition. W.H. Freeman and Co. (2009).
3. Murray, R. K., Granner, D. K., Mayes, P. A. & Rodwell, V. W. Harper's Illustrated Biochemistry. XXVIII edition. Lange Medical Books/ McGraw-Hill. (2009).

Course code: CH303

Course title: Analytical Methods in Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V

Module I: Qualitative and quantitative aspects of analysis: **(7 Lectures)**
Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Module II: Optical methods of analysis: **(11 Lectures)**
Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.
UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;
Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.
Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.
Structural illustration through interpretation of data, Effect and importance of isotope substitution.
Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Module III: Thermal methods of analysis: **(7 Lectures)**
Theory of thermogravimetry (TG), basic principle of instrumentation.
Techniques for quantitative estimation of Ca and Mg from their mixture.

Module IV: Electroanalytical methods: **(10 Lectures)**
Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points.
Techniques used for the determination of pKa values.

Module V: Separation techniques: **(10 Lectures)**
Solvent extraction: Classification, principle and efficiency of the technique.
Mechanism of extraction: extraction by solvation and chelation.
Technique of extraction: batch, continuous and counter current extractions.
Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.
Chromatography: Classification, principle and efficiency of the technique.
Mechanism of separation: adsorption, partition & ion exchange.
Development of chromatograms: frontal, elution and displacement methods.
Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.
Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).
Role of computers in instrumental methods of analysis.

Reference Books:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
2. Willard, H.H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C.: Exploring Chemical Analysis, 9th Ed. New York, W.H. Freeman, 2016.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age International Publisher, 2009.
6. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
7. Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
8. Ditts, R.V. Analytical Chemistry; Methods of separation, van Nostrand, 1974.

Course code: CH304
Course title: Industrial Chemicals and Environment
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry

Module-I: Industrial Gases and Inorganic Chemicals (10 Lectures)

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

Module-II: Industrial Metallurgy (5 Lectures)

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

Module-III: Environment and its segments (10 Lectures)

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO_2, CO_2, CO, NO_x, H_2S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Module-IV: Energy& Environment (10 Lectures)

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion/Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Module-V: Biocatalysis (8 Lectures)

Introduction to biocatalysis: Importance in "Green Chemistry" and Chemical Industry.

Reference Books:

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
4. S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
5. K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.
7. S. E. Manahan, Environmental Chemistry, CRC Press (2005).
8. G. T. Miller, Environmental Science 11th edition. Brooks/ Cole (2006).
9. A. Mishra, Environmental Studies. Selective and Scientific Books, New Delhi (2005).

Course code: CH305
Course title: Inorganic Materials of Industrial Importance
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry

Module-I: Silicate & Fertilizers Industries: (9 Lectures)

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses).
Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.
Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.
Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.
Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

Module-II: Surface Coatings: (9 Lectures)

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Module-III: Batteries & Alloys: (9 Lectures)

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.
Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Module-IV: Catalysis: (9 Lectures)

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.
Phase transfer catalysts, application of zeolites as catalysts.

Module-V: Chemical explosives: (9 Lectures)

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Reference Books:

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
7. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).

Course code: CH306R1
Course title: Molecular Modelling & Drug Design
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 4 T: 0 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Module I: Introduction to Molecular Modelling: [5]
Introduction. Useful Concepts in Molecular Modelling: 2D & 3D Molecular Structure, Configuration and Confirmation; Coordinate Systems; Potential Energy Surfaces; Molecular Graphics; Computer Hardware and Software.

Module II: Energy Minimization Methods and Introductory Statistical Mechanics: [10]
Minimization and related methods for exploring the potential energy surface. Non-derivative method, First and second order minimization methods. Simple thermodynamic properties and Phase Space. Concepts of Partition Function, Ensemble, Ergodic principle. Introduction to Error Analysis.

Module III: Molecular Dynamics & Monte Carlo Simulation: [10]
Concept of force field. Bond Stretching. Angle Bending, Torsion. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for Water. Periodic boundary condition. Minimum Image Convention. Integration Methods Used in Molecular Dynamics. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules.

Module IV: Basics of Electronic Structure Theory: [10]
a) Hartree-Fock (HF) Theory: Born-Oppenheimer approximation, Postulate of antisymmetry, Slater determinants, Slater-Condon rules for matrix elements, Hartree-Fock equations
b) Density Functional Theory (DFT): Introduction to electron density and functionals, Hohenberg Kohn Theorems, N- and V- representibility, Kohn-Sham equations, Discussion of some exchange-correlation functionals.
c) Elementary introduction to Basis sets.

Module V: Drug Design [10]
Ligand-Receptor Complex Based Drug Design, 3D Structural Understanding of Protein/Receptor Complex, X-Ray Cocrystal Structure of Protein-Ligand Complex and PDB database, 2D and 3D Ligand/Molecular Library Creation, Ligand-Receptor Interactions and Binding Mode Studies, Molecular Docking and Scoring.

Reference Books:
1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer – Anamaya Publishers, 2008.

Course code: CH307R1
Course title: Physical Chemistry-V Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

Phase Equilibria

I. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
a. simple eutectic and
b. congruently melting systems.
III. Distribution of acetic/ benzoic acid between water and cyclohexane.
IV. Study the equilibrium of at least one of the following reactions by the distribution method:
(i) $I_2(aq) + I^- \rightarrow I_3^-(aq)$
(ii) $Cu^{2+}(aq) + nNH_3 \rightarrow [Cu(NH_3)_n]^{2+}$

pH metry

V. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
VI. Preparation of buffer solutions of different pH
a. Sodium acetate-acetic acid
b. Ammonium chloride-ammonium hydroxide
VII. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
VIII. Determination of dissociation constant of a weak acid.

Reference Books

1. Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

Course code: CH308R1
Course title: Organic Chemistry-IV Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

A. *Chromatographic Separations*

1. TLC separation of a mixture containing 2/3 amino acids.
2. TLC separation of a mixture of dyes (fluorescein and methylene blue).
3. Column chromatographic separation of mixture of dyes.
4. Paper chromatographic separation of a mixture containing 2/3 amino acids.
5. Paper chromatographic separation of a mixture containing 2/3 sugars.

B. *Spectroscopic Analysis of Organic Compounds:*

1. Assignment of labelled peaks in the ^{1}H NMR spectra of the known organic compounds explaining the relative δ-values and splitting pattern.
2. Assignment of labelled peaks in the IR spectrum of the same compound explaining the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C≡C, C≡N stretching frequencies; **characteristic bending vibrations are included**).
3. The students must record full spectral analysis of **at least 15 (fifteen)** compounds from the following list: (i) 4-Bromoacetanilide (ii) 2-Bromo-4-methylacetophenone (iii) Vanillin (iv) 2-Methoxyacetophenone (v) 4-Aminobenzoic acid (vi) Salicylamide (vii) 2- Hydroxyacetophenone (viii) 1,3-Dinitrobenzene (ix) *trans*-Cinnamic acid (x) Diethyl fumarate (xi) 4-Nitrobenzaldehyde (xii) 4-Methylacetanilide (xiii) Mesityl oxide (xiv) 2-Hydroxybenzaldehyde (xv) 4-Nitroaniline (xvi) 2,3-Dimethylbenzonitrile (xvii) Pent-1-yn-3-ol (xviii) 3-Nitrobenzaldehyde (xix) 3-Aminobenzoic acid (xx) Ethyl-3-aminobenzoate (xxi) Ethyl-4-aminobenzoate (xxii) 3-Nitroanisole (xxiii) 4-Oxo-pentanoic acid (xxiv) Benzylacetate (xxv) Diethylmaleate.

Reference Books:

1. Manual of Biochemistry Workshop, Department of Chemistry, University of Delhi, 2012,
2. Arthur, I. V. Quantitative Organic Analysis, Pearson.

Course code: CH309
Course title: Lab: Analytical Methods in Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.

(ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the Rf values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their Rf values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

(i) To separate a mixture of Ni^{2+}& Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform, and determine its concentration by spectrophotometry.

(ii) Solvent extraction of zisconium with amberliti LA-1, separation from a mixture of irons and gallium.

3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.
4. Determination of Na, Ca, Li in cola drinks and fruit juices using fame photometric techniques.
5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of metal ions from their binary mixture.

(iii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry

1. Determination of pKa values of indicator using spectrophotometry.
2. Structural characterization of compounds by infrared spectroscopy.
3. Determination of dissolved oxygen in water.
4. Determination of chemical oxygen demand (COD).
5. Determination of Biological oxygen demand (BOD).
6. Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

Reference Books:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
2. Willard, H.H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, D.C. Exploring Chemical Analysis, 9th Ed. New York, W.H. Freeman, 2016.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Edition.
7. Mikes, O. & Chalmes, R.A. Laboratory Handbook of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
8. Ditts, R.V. Analytical Chemistry: Methods of separation. Van Nostrand, New York, 1974.

Course code: CH310
Course title: Lab: Industrial Chemicals and Environment
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-}, HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2.
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Reference Books:

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
4. S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
5. K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi.
6. S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.

Course code: CH311
Course title: Lab: Inorganic Materials of Industrial Importance
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 2
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

Reference Books:

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: Introduction to Ceramics, Wiley Publishers, New Delhi.
4. J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
5. P. C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi.
6. R. Gopalan, D. Venkappayya, S. Nagarajan: Engineering Chemistry, Vikas Publications, New Delhi.
7. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).

Course code: CH312
Course title: Lab: Molecular Modelling & Drug Design
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. V
Branch: Chemistry
Name of Teacher:

Syllabus

i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene.
Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N_2, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).
vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
ix. (a) Compare the optimized bond angles H_2O, H_2S, H_2Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.
x. Exploration of the potential energy surface of small molecules (H_2O, O_2, H_2S, N_2), geometry optimizations of ethane, ethene, ethyne and benzene, frequency calculation of ethane, ethene, ethyne and benzene.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, Gaussian.

Reference Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
3. Gupta, S.P. QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

Course code: CH 313R1
Course title: Inorganic Chemistry-IV
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry

Module I: Introduction to Organometallic complexes
Introduction, Classical and non-classically bonded organometallic compounds, 18 electron rule in Organometallic complexes-Ionic and Covalent Model; Metal Alkyls, Aryls, and Hydrides and Related σ-Bonded Ligands: Transition Metal Alkyls and Aryls, Related σ-Bonded Ligands, Metal Hydride Complexes, σ Complexes, Bond Strengths for Classical σ-Bonding Ligand;

Module II: Organometallic Compounds I (9 Lectures)
Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Module III: Organometallic Compounds II (9 Lectures)
Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls. Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler–Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Module IV: Reaction Kinetics and Mechanism (9 Lectures)
Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

Module V: Catalysis by Organometallic Compounds (9 Lectures)
Study of the following industrial processes and their mechanism:
1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes

Text books:
1. Svehla, G. Vogel's Qualitative Inorganic Analysis, 7th Edition, Prentice Hall, 1996.
2. Cotton, F. A. G.; Wilkinson & Gaus, P.L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
3. Huheey, J. E.; Keiter, E. A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
4. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
5. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry3rd Ed., John Wiley and Sons, NY, 1994.
6. Greenwood, N.N. & Earnshaw, A. Chemistry of the Elements, Elsevier 2nd Ed, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
7. Lee, J.D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
8. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
9. Shriver, D.D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
10. Basolo, F. & Pearson, R. Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.

Reference books:
1. Purcell, K.F. & Kotz, J.C., Inorganic Chemistry, W.B. Saunders Co. 1977

2. Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
3. Collman, J. P. et al. Principles and Applications of Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
4. Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000.
5. Spessard, G. O. & Miessler, G.L. Organometallic Chemistry. Upper Saddle River, NJ: Prentice-Hall, 1996.

Course code: CH 328
Course title: Organic Chemistry-V
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry

Module-1: The Logic of Organic Synthesis (10 lectures)

(i)*Retrosynthetic analysis:* Disconnections; synthons, donor and acceptor synthons; natural reactivity and *umpolung*; latent polarity in bifunctional compounds: illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and addition (FGI and FGA). (ii)*Strategy of ring synthesis:* Thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique. (iii) *Asymmetric synthesis*: Stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity Felkin-Anh model.

Module-2: Biomolecules. (13 lectures)

(i) *Aminoacids:* Synthesis with mechanistic details: Strecker, Gabriel; acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperizine, isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids. (ii) *Protein:* Peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using N-protection & C-protection, solid-phase (Merrifield) synthesis; peptide sequence: *C*-terminal and *N*-terminal Module- determination (Edman, Sanger and 'dansyl'methods); partial hydrolysis; specific cleavage of peptides; use of CNBr. Primary, secondary, tertiary and quaternary structure of proteins. Classification of proteins; Denaturation of proteins.(iii) *Nucleic acids:* Pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalysed hydrolysis of nucleosides; comparison of alkaline hydrolysis of DNA and RNA; complimentary base–pairing in DNA.

Module 3: Polynuclear hydrocarbon and their derivatives. (6 lectures)

Synthetic methods include Haworth, Bardhan-Sengupta, Bogert-Cook and other useful syntheses (with mechanistic details); fixation of double bonds and Fries rule; reactions (with mechanism) of naphthalene, anthracene and phenanthrene and their derivatives.

Module-4: Terpenoids, Steroids, Polyketide and Alkaloids. (12 lectures)

(I)Metabolites and classification of natural products; natural occurrence, general structural features, classification and importance of: (i) *Terpenoids* (geraniol, menthol and camphor), (ii) *Steroids* (Cholesterol, bile acids, androsterone, testosterone, estone, progesterone and aldosterone) (ii) Introduction to alkaloids, natural occurrence, general structural features and classification; Medicinal importance of Coniine, Nicotine, Atropine, Cocaine, Quinine, Chloroquine, Papaverine, Lysergic acid, Reserpine and Morphine. Synthesis of Nicotine, Quinine, Papaverine, Reserpine and Morphine

Module-5: Lipids and Flavonoids. (9 lectures)

(I)Lipids: Introduction and classification of lipids. Oils and fats: Common and naturally occurring fatty acids with structural features present in oils and fats, Omega fatty acids. Biological importance of triglycerides, phospholipids and glyco-lipids. (ii) *Flavonoids*: Introduction, structural features, classification and importance of flavonoids.

Text books:

1. Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
2. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
4. Solomons, G. T.W. Organic Chemistry, John Wiley & Sons, Inc.
5. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan (2010).
6. Kemp, W. Organic Spectroscopy, Palgrave.

Reference books:

1. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

2. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
3. Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
4. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India Ed., 2015.
5. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

Course code: CH315
Course title: Applications of Computers in Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 4 T: 0 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

Module I: Basics: (9 Lectures)

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions.

Module II:Elements of the BASIC language: (9 Lectures)

BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Module III: Numerical methods: (9 Lectures)

Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.
Differential calculus: Numerical differentiation.

Module IV: Integral calculus: (9 Lectures)

Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.
Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.
Interpolation, extrapolation and curve fitting: Handling of experimental data.

Module V: Conceptual background of molecular modelling: (9 Lectures)

Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Reference Books:

1. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5.
2. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
3. Noggle, J. H. Physical chemistry on a Microcomputer. Little Brown & Co. (1985).
4. Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).

Course code: CH316
Course title: Novel Inorganic Solids
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Module I: Synthesis and modification of inorganic solids: (9 Lectures)
Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

Module II: Inorganic solids of technological importance: (9 Lectures)
Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.
Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

Module III: Nanomaterials: (9 Lectures)
Overview of nanostructures and nanomaterials: classification.
Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires.
Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisical nanomaterials, bionano composites.

Module IV: Introduction to engineering materials for mechanical construction: (9 Lectures)
Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

Module V: Composite materials & Speciality polymers: (9 Lectures)
Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

Reference Books:

1. Shriver & Atkins. Inorganic Chemistry, Peter Alkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
2. Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry. John Wiley & Sons, 1974.
3. Poole, C.P. & Owens, F.J. Introduction to Nanotechnology John Wiley & Sons, 2003.
4. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.

Course code: CH317
Course title: Polymer Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Module I: Polymeric materials, its functionality and importance: (9 Lectures)
Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.
Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

Module II: Kinetics of Polymerization: (9 lectures)
Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

Module III: Nature and structural properties of polymers: (9 Lectures)
Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. Structure Property relationships.
(M_n, M_w, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.
Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

Module IV: Polymer Solution (8 Lectures)
Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

Module V: Properties of Polymers (Physical, thermal, Flow & Mechanical Properties) (10 Lectures)
Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

Reference Books:
1. R. B. Seymour & C.E. Carraher: Polymer Chemistry: An Introduction, Marcel Dekker, Inc. New York, 1981.
2. G. Odian: Principles of Polymerization, 4th Ed. Wiley, 2004.
3. F.W. Billmeyer: Textbook of Polymer Science, 2nd Ed. Wiley Interscience, 1971.
4. P. Ghosh: Polymer Science & Technology, Tata McGraw-Hill Education, 1991.
5. R.W. Lenz: Organic Chemistry of Synthetic High Polymers. Interscience Publishers, New York, 1967.

Course code: CH318R1
Course title: Instrumental Methods of Chemical Analysis
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry

Module I: Introduction to spectroscopic methods of analysis: (9 Lectures)
Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.
Infrared spectroscopy:
Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.
UV-Visible/ Near IR – emission, absorption, fluorescence and photoaccoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoaccoustic, fluorescent tags).
Module II: Separation techniques (9 Lectures)
Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.
Immunoassays and DNA techniques
Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).
Module III: Elemental analysis (9 Lectures)
Mass spectrometry (electrical discharges).
Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence.
Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).
Module IV: NMR spectroscopy: **(9 Lectures)**
Principle, Instrumentation, Factors affecting chemical shift, Spin-coupling, Applications.
Module V: Other Methods of Analysis: (9 Lectures)
Electroanalytical Methods**:** Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.
Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation).
Radiochemical Methods, X-ray analysis and electron spectroscopy (surface analysis**)**
Reference books:
1. D. A. Skoog, F. J. Holler & S. Crouch (ISBN0-495-01201-7) Principles of Instrumental Analysis, Cengage Learning India Edition, 2007.
2. Willard, Merritt, Dean, Settle, Instrumental Methods of Analysis, 7th ed, IBH Book House, New Delhi.
3. Atkins, P. W & Paula, J. D. Physical Chemistry, 10th Ed., Oxford University Press (2014).
4. Kakkar, R. Atomic and Molecular Spectroscopy: Concepts and Applications. Cambridge University Press, 2015.
5. Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
6. Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).

7. Smith, B. C. Infrared Spectral Interpretations: A Systematic Approach. CRC Press, 1998.
8. Moore, W.J., Physical Chemistry Orient Blackswan, 1999.

Course code: CH 319
Course title: Inorganic Chemistry-IV Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-},$S_2O_3^{2-}$, CH_3COO^-, F^-,Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+},, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+},Sr^{2+}, Ca^{2+}, Mg^{2+}
Mixtures should preferably contain one interfering anion, orinsoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) orcombination of anions e.g. CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible.
i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
iv. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
v. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Reference Books:

1. Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Pearson Education, 2002.
2. Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons 1972.

Course code: CH 320R1
Course title: Organic Chemistry-V Lab
Pre-requisite(s): Intermediate level Chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P:3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

Separation based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. $NaHCO_3$, *etc*., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture should be of the following types **[ANY THREE]**: *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotolune/*p*-Anisidine; benzoic acid/naphthalene; urea/phenyl benzoate; *p*-toluidine/benzophenone; *p*-chlorobenzoic acid/benzophenone, Benzoic acid/Anthracene; Glucose/Biphenyl; Benzoic acid/Benzophenone; Urea/Benzophenone. **Use of pH paper** is recommended.

Each student is required to perform all the experiments [Any **FIVE** will be set in the examination]

1. Estimation of glycine by Sörensen's formol method
2. Estimation of glucose by titration using Fehling's solution
3. Estimation of sucrose by titration using Fehling's solution
4. Estimation of aromatic amine (aniline) by bromination (Bromate-Bromide) method
5. Estimation of acetic acid in commercial vinegar
6. Estimation of urea (hypobromite method).
7. Estimation of saponification value of oil/fat/ester.

Determination of boiling point of common organic liquid compounds [**ANY FIVE**]*n*-butyl alcohol, cyclohexanol, ethyl methyl ketone, cyclohexanone, acetylacetone, isobutyl methyl ketone, isobutyl alcohol, acetonitrile, benzaldehyde and acetophenone. [Boiling points of the chosen organic compounds should preferably be within 180°C (Demo)].

Reference Books:

1. Vogel, A. I. Quantitative Organic Analysis, Part 3, Pearson (2012).
2. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry, Pearson Education (2009)
3. Furniss, B. S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
4. Ahluwalia, V. K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
5. Ahluwalia, V. K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

Course code: CH 321
Course title: Lab: Applications of Computers in Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Simple exercises using molecular visualization software.

Reference Books:

1. McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
2. Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
3. Steiner, E. The Chemical Maths Book Oxford University Press (1996).
4. Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007).
5. Harris, D. C. Quantitative Chemical Analysis. Chapters 3-5, 6th Ed., Freeman (2007).
6. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, 487 pages, Cambridge Univ. Press (2001).
7. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).
8. Venit, S.M. Programming in BASIC: Problem solving with structure and style. Jaico Publishing House: Delhi (1996).

Course code: CH 322
Course title: Lab: Novel Inorganic Solids
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

1. Determination of cation exchange method
2. Determination of total difference of solids.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

Reference Book:

1. Fahlman, B. D. Materials Chemistry, Springer, 2004.

Course code: CH 323
Course title: Lab: Polymer Chemistry
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

1. **Polymer synthesis**

1. Free radical solution polymerization of styrene (St)/Methyl Methacrylate (MMA)/Methyl Acrylate (MA)/Acrylic acid (AA).
a. Purification of monomer
b. Polymerization using benzoyl peroxide (BPO)/2,2'-azo-bis-isobutylonitrile (AIBN)
2. Preparation of nylon 66/6
1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
a. Preparation of IPC
b. Purification of IPC
c. Interfacial polymerization
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:
(a) Polyacrylamide-aq.$NaNO_2$ solution
(b) (Polyvinyl proplylidine (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis

*at least 7 experiments to be carried out.

Reference Books:

1. M.P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed., Oxford University Press, 1999.
2. H.R. Allcock, F.W. Lampe & J.E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
3. F.W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
4. J.R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
5. P. Munk & T.M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
6. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
7. M.P. Stevens, Polymer Chemistry: An Introduction 3rd ed. Oxford University Press (2005).
8. Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

Course code: CH 324
Course title: Lab: Instrumental Methods of Chemical Analysis
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: I. M. Sc.
Semester / Level: I. M. Sc. VI
Branch: Chemistry
Name of Teacher:

Syllabus

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)
8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride)
10. Separation of Carbohydrates by HPLC
11. Determination of Caffeine in Beverages by HPLC
12. Potentiometric Titration of a Chloride-Iodide Mixture
13. Cyclic Voltammetry of the Ferrocyanide/ Ferricyanide Couple
14. Nuclear Magnetic Resonance
15. Use of fluorescence to do “presumptive tests” to identify blood or other body fluids.
16. Use of “presumptive tests” for anthrax or cocaine
17. Collection, preservation, and control of blood evidence being used for DNA testing
18. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y chromosome only or multiple chromosome)
19. Use of sequencing for the analysis of mitochondrial DNA
20. Laboratory analysis to confirm anthrax or cocaine
21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

At least 10 experiments to be performed.

Reference Books:

1. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
2. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.

Course code: CH 401
Course title: Inorganic Chemistry-V: Basic Inorganic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:

Syllabus

Module I: Chemical Bonding: Valency Theories- Quantum Chemical Approach (9 Lectures)

Huckel approximation applied to H_2^+ and H_2 type systems, comparative study of the application of VB and MO methods to diatomic (homo and hetero) species; MO of polyatomic molecules; Walsh diagram, configuration interaction, orbital construction for Hn type systems, localized and delocalized M.O., σ, π, δ bonds, polyatomic molecules, electron deficient and hypervalent molecules.

Module II: Quantitative basis of Crystal Fields (9 Lectures)

Crystal Field Theory, The octahedral Crystal Field potential, The effect of V_{oct} on the *d* wave-functions, the evaluation of Δ, The tetrahedral and cubic potentials. Energy level of transition metal ions, Effect of ligands fields on the energy levels of trasition metal ions.

Module III: Reaction Mechanism of Transition Metal Complexes (9 Lectures)

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valency bond and crystal field theory, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, substitution reaction in square complexes, trans effect, redox reactions, electron transfer reactions, mechanism of one electron transfer reaction, outer sphere type reactions, inner sphere type reactions.

Module IV: Introduction to electronic Spectra of transition metal complexes (9 Lectures)

Important features of transition metal electronic spectra- band intensities, band energies, band width and sets; characteristic spectra of complexes of fast row transition metal ions, Octahedral, tetrahedral and square planar complexes of first row transition metal ions; Effect of temperature on electronic bands, Spectrochemical & Nephelauxetic series.

Module V: Theoretical basis of Electronic Spectra of transition metal complexes (9 Lectures)

Spectroscopic ground state, Orgel and Tanabe–Sugano diagrams for transition metal complexes, calculations of D_q, B and beta parameters, Charge transfer spectra: Intraligand charge transfer spectra, Metal to ligand charge transfer spectra, Ligand to metal charge transfer spectra Absorption spectra of *f*-block elements.

Text books:

1. G. Wulfsberg, Inorganic Chemistry, University Science Books, 2000.
2. C. J. Ballhausen & H. B. Gray, Molecular Orbital Theory, W.A. Benjamin, 1978.
3. F. Basolo & R. G. Pearson, Inorganic Reaction Mechanism, 2nd ed., John Wiley & Sons Inc., 1967.
4. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsvier, 1984.

Reference books:

1. B. N. Figgis and M. A. Hitchman, Ligand Field Theory and its Applications, Wiley–VCH, New York, 2000.
2. I. B. Bersuker, Electronic Structure and Properties of transition metal compounds, 2nd ed., Wiley, 2010.
3. C. J. Ballhausen, Introduction to Ligand Field Theory, McGraw-Hill Inc., 1962.
4. R. B. Jordon, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd ed., Oxford Unversity Press, 2007.
5. D. N. Sathyanarayana, Electronic Absorption Spectroscopy, Universities Press, 2001.
6. E. A. B. Ebsworth, D. W. H. Rankin, S. Cardock, Structural Methods in Inorganic Chemistry; 2nd ed., Wiley-Blackwell, 1991.
7. A. K. Das, M. Das, Fundamental Concepts of Inorganic Chemistry; Volume-1-5; CBS Publishers, 2012.
8. R Sarkar, General and Inorganic Chemistry- Volume-I and Volume-II, 3rd revised ed., New Central Book Agency, 2011.

Course code: CH402R1
Course title: Physical Chemistry-VI: Chemical Kinetics & Surface Chemistry
Pre-requisite(s): B.Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:
Course Objectives

Module I: Chemical Reaction Dynamics (10 lectures)
Introduction to reaction kinetics; Linear and non-linear Arrhenius equation, Thermodynamic treatment of bimolecular gaseous reactions (Eyring equation). Theories of unimolecular gaseous reactions: Lindemann-Hinshelwood, RRK and RRKM theories. Kinetics of reactions in solution. Kinetics of fast reactions: Relaxation method, Flow methods, Pulse methods, flash photolysis. Molecular reaction dynamics, potential energy surfaces. Electron transfer reactions. Heterogeneous catalysis: Kinetics of surface reactions unimolecular and bimolecular. Autocatalysis and oscillatory reactions.

Module II: Electrochemistry (10 lectures)
Debye-Hückel theory of ion-ion interaction and activity coefficient, Applicability and limitations of Debye-Hückel limiting law, its modification, Effect of ion-solvent interaction on activity coefficient. Thermodynamic treatment of electrified interfaces, Introduction to electrical double layer, Introduction to electrode kinetics: Butler-Volmer equation, polarography, cyclic voltammetry, corrosion, fuel cells.

Module III: Photochemistry (10 lectures)
Consequences of light absorption; Kinetics of photochemical reactions: H_2-Br_2, H_2-Cl_2 & decomposition of HI. Potential energy diagram, Franck-Condon principle. Photophysical processes: fluorescence, phosphorescence, delayed fluorescence. Photophysical kinetics of unimolecular processes. Bimolecular collisions in gases and vapours and the mechanism of fluorescence quenching. Kinetics of collisional quenching: Stern-Volmer equation. Techniques for the study of transient species in photochemical reactions. Lasers in photochemical kinetics.

Module IV: Surface Chemistry: (9 lectures)
Adsorption by solids-types and applications. Adsorption of gases by solids. Adsorption isotherms: Freundlich and Langmuir adsorption isotherms, BET theory of multilayer adsorption, Types of adsorption isotherms. Adsorption from solution: Gibb's adsorption isotherm. Modern techniques for investigating surfaces.

Module V: Colloidal States: (6 lectures)
Basics of colloidal states, electrical and electrokinetic properties, Micelles: Surface active agents, Classifications, micellization, hydrophobic interaction, CMC, factors affecting the CMC surfaces, counter ion binding, Thermodynamics of micellization-phase separation, solubilization, Micro-emulsion, Reverse micelles

Text books:
1. P. Atkins and J. Paula, Physical Chemistry, 10th ed., Oxford University Press, Oxford, 2014.
2. K. J. Laidler, Chemical Kinetics, 3rd ed., Harper & Row, New York, 1998.
3. J. O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 2, 2nd ed., Plenum Press, New York, 1998.
4. K. K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International Pvt. Ltd.; 3rd ed., New Delhi, 2014.
5. A. W. Adamson and A. P. Gast, Physical Chemistry of Surfaces, 5th ed., Wiley, 1997.

Reference books:
1. M. R. Wright, An introduction to chemical kinetics, 1st ed., Wiley, 2005.
2. I. N. Levine, Physical Chemistry, 5th ed., 2002.
3. M. J. Pilling and A. P.W, Seakins, Reaction Kinetics, Oxford Science Publication, New York, 1998.
4. J. G. Calvert and J. N. Pitts, Jr., Photochemistry, John Wiley & Sons, New York, 1966.
5. R. P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, Oxford, 1988.
6. J. I. Steinfeld, J. S. Francisco, W. L. Hase, Chemical Kinetics and Dynamics, 2nd ed., Pearson, 1998.
7. M. Satake, S. A. Iqbal, Colloidal & Surface Chemistry, Discovery Publishing Pvt. Ltd, 2003.

Course code: CH403R1
Course title: Reaction Mechanisms in Organic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:

Module I: Aliphatic substitution reactions [10 Lectures]
Nucleophilic substitution: The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms, neighbouring group participation by pi and sigma bonds, anchimeric assistance, The S_Ni mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium; Electrophilic bimolecular mechanism-S_E2 and S_Ei: The S_E1 mechanism, electrophilic substitution accompanied by double bond shift, effect of substrates, leaving group and the solvent polarity on the reactivity.

Module II: Aromatic substitution reactions [10 Lectures]
The arenium ion mechanism, orientation and reactivity, energy profile diagrams, The*ortho*/*para* ratio, ipso attack, Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction, The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms, Reactivity–effect of substrate structure, leaving group and attacking nucleophile, The Von Richter, Sommelet-Hauser, Smiles Rearrangement.

Module III: Addition and Elimination Reactions [10 Lectures]
Mechanism and stereochemical aspects of addition reaction in carbon-carbon and carbon-hetero multiple bonds, regio-and chemoselectivity, orientation and reactivity, Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions.
The E2, E1 and E1cB mechanism and their spectrum, orientation of the double bond, Reactivity- effect of substrates structure, attacking base, the leaving group and the medium, Mechanism and orientation in pyrolytic elimination.

Module IV: Rearrangement Reaction [10 Lectures]
General Mechanistic considerations – nature of migration, migratory aptitude, A detailed study of the following rearrangements involving carbonation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), reaction involving acyl cation, PPA cyclization and Fries rearrangement, rearrangement of carbenes (Wolff & Arndst-Eistert synthesis), rearrangement of nitrenes (Hoffman, Curtius, Schmidt, Lossen, Beckman rearrangement).

Module V: Concerted reactions [10 Lectures]
FMO & PMO approach, frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, allyl system, FMO approach, types of cyclo-additions and cyclo-reversion reactions, electrocyclic reaction and the electroreversion reactions, sigmatropic reactions, group transfer reaction. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 Cyloaddition Reaction: Antarafacial and suprafacial additions, 4n and 4n+2 systems, Diels-Alder Reaction, Stereo selectivity and Regioselective Diels-Alder Reactions, Sigmatropic rearrangements: Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties.

Text books:
1. I. L. Finar, Organic Chemistry, Vol. I and II, 5th ed., Longman Ltd., New Delhi, 2011.
2. P. Sykes, A Guide Book to Mechanism in Organic Chemistry, 6th ed., John Wiley & Sons, New York, 1985.
3. T. W. G. Solomons, Fundamentals of Organic Chemistry, 4th ed., John Wiley, 1994.
4. R. N. Morrison & R. N. Boyd, Organic Chemistry, 7th ed., Dorling Kindersley (India) Pvt. Ltd. (Pearson Education), 2010.

Reference books:
1. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 2nd ed., Oxford Press, 2012,
2. J. March, Organic reaction and mechanism-structure and reactivity, 7th ed., John Wiley, 2015.
3. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, New York, 2006.

Course code: CH404R1
Course title: Inorganic Chemistry-VI: Organometallic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:
Course Objectives

Syllabus

Module I: Organometallic Complexes: General properties and types (9 Lectures)

Complexes of π-Bound Ligands: Alkene and Alkyne Complexes, Allyl Complexes, Diene Complexes, Cyclopentadienyl Complexes, Arenes and Other Alicyclic Ligands, Metalacycles and Isoelectronic and Isolobal Replacement, Stability of Polyene and Polyenyl Complexes.

Module II: Metal–Ligand Multiple Bonds (9 Lectures)

Carbenes: Fischer Versus Schrock Carbenes - conditions, synthesis examples reactivity and structure, Cases Intermediate Between Fischer and Schrock Carbenes, Boryl Complexes, Vinylidene Carbynes-synthesis, examples and reactivity, structure, Bridging Carbenes and Carbynes, N-Heterocyclic Carbenes-synthesis examples reactivity and structure, Multiple Bonds to Heteroatoms.

Module III: Reactivity of Organometallic Complexes: I (9 Lectures)

Oxidative Addition and Reductive Elimination: Concerted Additions, S_N2 Reactions, Radical Mechanisms, Ionic Mechanisms, Reductive Elimination, σ-Bond Metathesis, Oxidative Coupling and Reductive Cleavage.

Insertion and Elimination: Reactions Involving CO, Insertions Involving Alkenes, Other Insertions, α, β, γ, and δ Elimination.

Module IV: Reactivity of Organometallic Complexes: II (9 Lectures)

Nucleophilic and Electrophilic Addition and Abstraction: Nucleophilic Addition to CO, Nucleophilic Addition to Polyene and Polyenyl Ligands, Nucleophilic Abstraction in Hydrides, Alkyls and Acyls, Electrophilic Addition, Electrophilic Abstraction of Alkyl Groups, Single-Electron Transfer Pathways, Reactions of Organic Free Radicals with Metal Complexes.

Homogeneous Catalysis: Alkene Isomerization, Alkene Hydrogenation, Alkene Hydroformylation, Hydrocyanation of Butadiene, Alkene Hydrosilation and Hydroboration, Coupling Reactions, Surface and Supported Organometallic Catalysis.

Module V: Applications of Organometallic Chemistry (9 Lectures)

Alkene Metathesis- mechanism, Type and commercial application, Dimerization, Oligomerization, and Polymerization of Alkenes- mechanism, Type and commercial application, Activation of CO and CO_2 - mechanism, Type and commercial application, CH Activation- mechanism, Type and commercial application, Organometallic Materials and Polymers.

Text books:

1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience; 4th ed., 2005.

Reference books:

1. B- M. Bochmann, Organometallic Chemistry: (Oxford series), 1994.
2. R. C. Mehrotra & A. Singh, Organometallic Chemistry, New Age Int. Publishers, 2nd ed., 1991.
3. M. Gielen, R. Willem, B. Wrackmeyer, Fluxanol Organometallic and Coordination compounds, Wiley, 1st ed., 2008.
4. F. A. Cotton, G. Willkinson, Advanced Inorganic Chemistry,Wiley, 6th ed., 2007.
5. J. E. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 4th ed. 2006.

Course code: CH405R1
Course title: Principles of Organic Synthesis
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:

Module I: Conformation and Reactivity [10 Lectures]
Conformation around sp^3-sp^2 and sp^2-sp^2 bond, conformation around carbon hetero atom bond, conformations of cyclic system (cyclopentane, cyclohexane with mono and di substituted cyclohexanes, cycloheptane, cyclooctane and decalins),, Conformation of cyclohexane, monosubsituted, disubstituted, etc. Reactivity of cyclohexane and substituted system (substitution, addition, elimination, rearrangement etc.).

Module II: Principles of Organic Reaction [10 Lectures]
Reagent type and reaction type, Investigation of reaction mechanism (nature of products, kinetic data, use of isotope, study of intermediate, stereochemical criteria.Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, free energy relationships, kinetic and thermodynamic control, Nature of reaction energy, Potential energy diagrams, transition states and intermediates, methods of determing mechanisms, nonkinetic methods of determining reaction mechanism, isotope effects, solvent effect.

Module III: Principles of Reaction Mechanism [10 Lectures]
Hammond's postulate, Curtin-Hammett principle, Hammett energy diagrams and reaction rate laws, Hammett's σ_x and ρ values and their physical significance through-conjugation, deviations from straight line plots; steric effects: Taft equation, Softness (Hardness) Scales, HSAB principle, HSAB application for organic reactions: Reaction Selectivity, Alkylation vs. Acylation, C- vs. O-Alkylation, Reactions of Organosulfur Compounds, Reactions of Organophosphorus Compounds, Elimination and Substitution, Addition to Double Bonds, Addition to Carbonyl Compounds.

Module IV: Asymmetric synthesis (10 Lectures)
Stereoisomerism, methods of resolution, optical purity, prochirality, enantiotopic and diastereotopic atoms, groups and faces, optical activity Cram's rule, Felkin's rule, Prelog's rule, Karabatso's rule and their application in organic synthesis (stereoselectivity in hydride reduction), Homogenous and heterogenous asymmetric catalysis.

Module V: Principles of Retrosynthesis (10 Lectures)
Methodologies in organic synthesis-basic ideas on synthons and synthetic equivalents, disconnection approach, functional group transformations and inter-conversions of simple functionalities, Disconnection Approaches, Functional Group Interconversions (FGI). Concept of synthetic efficiency: one pot, multi-component and atom economical reactions. linear and convergent synthesis. One group disconnections, Reactions examples One group C-C and C-X disconnection, Umpolung of reactivity and protecting groups. Two group C-C disconnections, Diels-Alder reaction,

Text books:
1. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 2nd ed., Oxford Press, 2012.
2. I. L. Finar, Organic Chemistry, Vol. I & II, 5th ed., Longman Ltd., New Delhi, 2011.
Reference books:
1. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th ed., John Wiley & Sons, New York, 1985.
2. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd ed., New Age Int., New Delhi, 1994.
3. I. Fleming, Pericyclic Reactions, Oxford Scientific Publication, Cambridge, 1998.
4. E. V. Anslyn and D.A. Dougherty, Modern Physical Organic Chemistry, University Science Books, USA, 2006.
5. L. P. Hammett, Physical Organic Chemistry, 1st ed., McGraw-Hill Book Co. Inc., New York, 1940.

Course code: CH 406
Course title: Physical Chemistry-VI Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: M. Sc. and I. M.Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:

Syllabus

Adsorption: (any two)

(i) To study surface tension-concentration relationship for solutions.
(ii) To study the adsorption of iodine from alcoholic solution of charcoal.
(iii) To study the adsorption of acetic acid on charcoal.

Chemical equilibrium: (any one)

(i) To determine congruent composition & temperature of a binary system- Phenol-water.
(ii) To determine glass transition temperature of a given salt conductometrically.
(iii) To construct the phase diagram for a three component systems.
(iv) To determine the equilibrium constant for the reaction $KI + I_2 = KI_3$.

Chemical Kinetics: (any two)

(i) To determine rate constant of saponification ethyl acetate by NaOH.
(ii) To determine the velocity constant of hydrolysis of an ester in micellar media.
(iii) To determine the rate constant for the oxidation of iodide ion by hydrogen peroxide, studying the kinetics as an iodine clock reaction.

Conductometry: (any two)

(i) To determine velocity constant, order of reaction and energy of activation for saponification of ethyl acetate by NaOH conductometrically.
(ii) To determine solubility and solubility product of sparingly soluble salt conductometrically.
(iii) To determine the strength of strong and weak acids in a given mixture conductometrically.
(iv) To determine activity co-efficient of zinc ions in the solution of 0.002 M $ZnSO_4$ using Debye-Huckel's limiting law.

Potentiometry-pH metry: (any one)

(i) To determine the strengths of halides in a mixture potentiometrically.
(ii) To determine the valancy of mercurous ions potentiometrically.
(iii) To determine the strength of strong and weak acids in a given mixture using a potentiometer-pH meter.
(iv) To determine the temperature dependence of E.M.F. of a cell.
(v) Acid-base titration in a non-aqueous media using a pH meter.
(vi) To determine the transport number by Hittrof's method.

Cyclic voltametry:

(i) To find the redox potential of the given sample using cyclic voltametry.

Polarography: (one one)

(i) To determine DO in aqueous solution of organic solvent
(ii) To determine half way potential of Cd & Zn EMF:
(iii) To determine single electrode potential of Cu/Cu^{2+}
(iv) Potentiometric titration of a redox system.
(v) To determine E.M.F. of concentration cell.

Polarimetry: (any one)

(i) To determine rate constant for hydrolysis/inversion of sugar using a Polarimeter.
(ii) Enzyme kinetics-inversion of sucrose.

Spectroscopy: (any one)

(i) To determine pK_a of an indicator in aqueous and micellar medium.
(ii) To determine stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (amine-iodine) complexes.

Thermochemistry: (any one)

(i) To determine the enthalpy of neutralization of hydrochloric acid with NaOH
(ii) Enthalpy of combustion of benzoic acid using DSC.

Text books:

1. J. B. Yadav, Advanced Practical Physical Chemistry, 22nd ed., Goel Publishing House, Krishna Prakashan Media, 2014.
2. B. Viswanathan and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2012.

Reference books:

1. B. P. Levitt, Findlay's Practical Physical Chemistry, 9th ed., Longman, London, 1985.
2. A. M. Halpern and G. C. McBane, Experimental Physical Chemistry: A Laboratory Text Book, 3rd ed., W. H. Freeman, 2006.
3. A. M. James and F. E. Prichard, Practical Physical Chemistry, Prentice Hall Press, 1974.

Course code: CH 407
Course title: Organic Chemistry-VI Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: I. M. Sc. and M.Sc.
Semester / Level: M. Sc. I/ I. M. Sc. VII
Branch: Chemistry
Name of Teacher:

Syllabus

1. Identification of functional groups through qualitative analysis in a given binary mixture of organic compounds.
2. Isolation of the organic compounds from above mentioned binary mixture through solvent extraction and verifying their complete separation through thin layer chromatography.
3. Identification of the isolated organic compounds through derivative preparation and characterization by FTIR, UV-VIS & NMR.
4. Electrophilic aromatic substitution: acylation of bromobenzene and checking thin layer chromatography to check the reaction outcome (product distribution and extent of reaction).

Reference Books:

1. A. I. Vogel, Quantitative Organic Analysis, Part 3, Pearson, 2012.
2. F. G. Mann, & B. C. Saunders, Practical Organic Chemistry, Pearson Education, 2009.
3. B.S. Furniss, A. J. Hannaford, P.W.G. Smith, A. R. Tatchell, Practical Organic Chemistry, 5th Ed., Pearson, 2012.
4. V.K. Ahluwalia, & R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2000.
5. V. K. Ahluwalia, & S. Dhingra, Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press, 2000.

Course code: CH 408
Course title: Inorganic Chemistry-VII: Advanced Inorganic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Syllabus

Module I: Magnetic properties of coordination Complexes (9 Lectures)

Definition of magnetic properties, Types of magnetic bodies, Experimental arrangements for the determination of magnetic susceptibility: Guoy method, Faraday method, Vibrating sample magnetometer, SQUID, NMR method; Diamagnetism in atoms and polynuclear systems, Pascals constant, Two sources of paramagnetism.

Module II:Thermal energy and magnetic properties (10 Lectures)

Spin & Orbital effects, Spin orbit coupling, Lande interval rule, Energies of J levels, Multiplet width and temperature; Curie equation, Curie & Curie–Weiss law, 2nd order Zeeman Effect, Temperature independent paramagnetism, Van Vleck susceptibility equation, Thermal Equillibrium between High Spin and Low spin state in Spin Cross over region, Magnetic behavior of lanthanides & actinides, Anomalous magnetic moments, magnetic properties of binuclear and polynuclear complexes— ferromagnetism and anti-ferromagnetism.

Module III: Anamolous Magnetic Moments in Coordination Complexes (9 Lectures)

Superexchange interaction in terms of Goodenough-Kanamori-Anderson Rules (GKA Rules), Interpretation of magnetic exchange by GKA Rule in terms of Molecular Orbital Theory, Antiferromagnetism in magnetically concentrated system, Cooperative magnetic interactions in binuclear Cu(II) complexes, Antiferromagnetic coupling in other metal complexes: Dimers of oxidovanadium(IV) and oxidomolybdenum(V) complexes, Dinuclear complexes of Ti(III), Dimeric Cr(II) acetate- monohydrate, $Mn_2(CO)_{10}$

Module IV: Inorganic Rings and Cages (8 Lectures)

Rings: Homocyclic rings of S, Se and Te. Heterocyclic rings of S, N, P and O; Cages: Higher boron hydrides: structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes.

Module V: Inorganic Cluster (9 Lectures)

Clusters in elemental states, cluster classification, Low nuclearity ($M_3 – M_4$) and high nuclearity cluster ($M_5 – M_{10}$), Metal metal bonding (MOT), Carbonyl clusters, skeletal electron counting, Wade-Mingos-Luber rule, application of isolobal and isoelectronic analogy, capping rules, carbide, nitride, chalcogenide and halide containing cluster of Re, Nb, Ta, Mo, W.Zintl ions, chevrel compounds, infinite metal chains, application of cluster compounds in catalysis.

Text books:

1. F. A. Cotton, G. Willkinson, Advanced Inorganic Chemistry,Wiley, 6th ed., 2007.
2. J. E. Huheey, Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 4th ed. 2006.
3. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, East-West Press, 1993.
4. A. K. Das, M. Das, Fundamental Concepts of Inorganic Chemistry; Volume-6; CBS Publishers, 2012.

Reference books:

1. G. Wilkinson, R. D. Gillars & J. A. Mccleverty, Comprehensive Co-ordination Chemistry, 2nd ed., Elsvier, 2003.
2. J. D. Lee, Concise Inorganic Chemistry, 5th ed., Oxford, 2008.
3. F. E. Mabbs and D. J. Machin, Magnetism and Transition Metal complexes, Dover Publications; 2008.
4. N. N. Greenwood and E. A. Earnshaw; Chemistry of elements, 2nd ed., Butterworth- Heinemann, 1997.

Course code: CH 409
Course title: Physical Chemistry-VII: Quantum Chemistry & Group Theory
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Module I: Classical Mechanics and Postulates of Quantum Mechanics (9 lectures)
Postulates of quantum mechanics. Operators in quantum mechanics: Linear and Hermitian operators, operator algebra, eigenvalues and eigenfunctions, commutation relations. Solution of Schrödinger's equation for (i) particle in 3D-boxes and applications, (ii) particle in a ring and sphere, spherical harmonics, angular momentum rigid rotator, (iii) Simple harmonic oscillator, and (iv) Hydrogen atom. Stark and Zeeman effect.

Module II: Approximation Methods (8 lectures)
Perturbation (Time-independent & Time-dependent) and Variation methods: Examples of Variation methods: (i) Hydrogen atom, Hydrogen atom in an electric field, (ii) Helium atom. Examples of Perturbation method: (i) perturbed particle in a box, (ii) perturbed harmonic oscillator (iii) Hydrogen atom in electric field.

Module III: Atomic Spectra and Atomic Structure (9 lectures)
The spectrum of atomic hydrogen: Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, spin-orbit coupling, selection rules for atomic spectra; The structure of helium; Many-electron atoms: Antisymmetric wave functions of many electron atoms, Slater determinants, Hartree and Hartree-Fock self-consistent field model for atoms.

Module IV: Theory of Angular Momentum & Chemical Bonding (9 lectures)
Angular momentum: Classical & quantum mechanical concept, application in many-electron atom, splitting of term level into atomic levels. *Molecular structure & Chemical bonding*: Born–Oppenheimer approximation, Hydrogen molecule ion. LCAO–MO and VB treatments of the hydrogen molecule. Hybridization and MOT of H_2O, NH_3 and CH_4. Huckel pi-electron theory and its applications to ethylene, butadiene and benzene.

Module V: Basic Concept of Symmetry & Group Theory (10 lectures)
Definition and theorem of group theory. Molecular symmetry & the symmetry group: Symmetry operations & symmetry elements, classification of molecules, multiplication tables. Representation of molecular point groups, character, reducible and irreducible representations. The Great Orthogonality Theorem (GOT, without proof), use of GOT to construct character table, character table for point groups & their uses.

Text books:
1. P.W. Atkins and R.S. Friedman, Molecular Quantum Mechanics, 4th edition, Oxford University Press. Oxford, 2005.
2. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983.
3. R. K. Prasad, Quantum Chemistry, 3rd ed., New Age International, 2006.
4. A. K. Chandra, Introductory Quantum Chemistry, Tata Mcgraw-Hill, New Delhi, 1988.
5. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 1996.

Reference books:
1. H. Eyring, J.Walter and G. E. Kimball, Quantum Chemistry, John Wiley, New York, 1944.
2. I. N. Levine, Quantum Chemistry, 5th ed., Pearson Educ., Inc., New Delhi, 2000.
3. D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Education, 2005.
4. J. P. Lowe and K. A. Peterson, Quantum Chemistry, 3rd ed., Academic Press, 2005.
5. D. M. Bishop, Group theory and Chemistry, Dover, 1993.
6. S. N. Datta, Lectures on Chemical bonding and quantum chemistry, Prism Books, Bangalore, 1997.

Course code: CH 410R1
Course title: Modern Organic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Module I: Protection and deprotection (10 Lectures)

Principle of protection and deprotection of alcohol, amine, carbonyl and carboxyl groups

Module II: Organic Photochemistry (10 Lectures)

Singlet and triplet excited state, radiative and non-radiative transitions, potential energy surfaces, photoreduction, photoaddition, photorearrangement, photooxidation, aromatic substitution, Norrish Type I, Norrish Type II, excimers and exciplexes, photochemistry of alkenes, carbonyl, aromatic compounds.

Module III: Free Radical Reaction (10 Lectures)

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, Reactivity for aliphatic and aromatic substrates, Reactivity in the attacking radicals, the effect of solvents on reactivity, Allylic halogenation, Oxidation of aldehydes to carboxylic acids, auto-oxidation, Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

Module IV: Neighboring Group Participation (10 Lectures)

Concept of neighboring group participation with mechanism, neighboring group participation by π & σ bonds, classical and non-classical carbocations, Intramolecular displacement by hydrogen, Oxygen, nitrogen, sulphur and halogen. Anchimeric assistance using Alkyl, cycloalkyl, Aryl participation, participation in bicyclic system, migratory aptitude, intimate and solvent separated ion-pair, transannular, pinacole and carbocation rearrangements and related rearrangements in neighboring group participation, NGP in elimination and addition.

Module V: Organometallic reagents (10 Lectures)

Principle, preparations, properties and applications of the following reagents in organic synthesis with Mechanistics details: Group – I & II metal organic compounds-Li, M, Hg, Cd, Zn & Ce compounds. Transition metals – Cu, Pd, Ni, Fe, Co, Rh, Cr & Ti compounds.

Text books:

1. J. March, M. B. Smith, Advanced Organic Chemistry – Reactions, Mechanism and Structure, 7th ed., John Wiley, 2015.
2. S. M. Mukherjee, Pericyclic Reactions: A Mechanistic Study, 3rd ed., Macmillan, India, 2010.
3. I. L. Finar, Organic Chemistry, Vol. I & II, 5th ed., Longman Ltd., New Delhi, 2011.
4. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd ed., New Age Int., New Delhi, 1994.

Reference books:

1. T. H. Lowry and K. S. Richardson, Mechanisms and Theory in Organic Chemistry, 2nd ed., Harper and Row, New York, 1981.
2. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, Springer, New York 2006.
3. I. Fleming, Frontier orbitals and organic chemical reactions, John Wiley and sons, Student edition, 2009.

Course code: CH411
Course title: Physical Chemistry-VIII: Equilibrium, Non-Equilibrium & Statistical Thermodynamics
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 3 L: 3 T: 0 P: 0
Class schedule per week: 03
Class: M. Sc. and I. Msc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Module I: Equilibrium Thermodynamics Basics (8 lectures)
Introduction to thermodynamics: Concept of work and heat, first law of thermodynamics, enthalpy and heat capacities, concept of entropy, residual entropy. Maxwell's relations and its applications and thermodynamic equations of state.
Module II: Equilibrium Thermodynamics Applications (9 lectures)
Free energy, free energy of mixing of gases, Gibbs-Helmholtz equations with its applications. Chemical potential, determination of partial molar quantities; Clapeyron-Clausius equation, fugacity & activity of gas and liquid. Third law of thermodynamics: Determination of absolute entropy of solids, liquids & gases, Boltzmann entropy equation.
Module III: Statistical Thermodynamics Basics (8 lectures)
Concept of distribution, Thermodynamic probability and most probable distribution, Maxwell-Boltzmann statistics, Bose-Einstein statistics, Fermi-Dirac statistics. Ensemble averaging, Canonical, Grand canonical and micro canonical ensembles.
Module IV: Statistical Thermodynamics Applications (10 lectures)
Ideal Gases: Partition functions: Translational, rotational, Vibrational and electronic partition functions and calculation of thermodynamic properties in terms of partition functions for ideal monatomic and diatomic gas. Equilibrium constant of an ideal gas reaction in terms of partition function. *Real gases:* intermolecular potential and virial coefficients. Debye and Einstein theory of heat capacity of solids. Structure and thermal properties of liquids, Pair correlation functions. *Solids:* Thermodynamics of solids - Einstein and Debye models. T^3 dependence of heat capacity of solids at low temperatures (universal feature). *Metals:* Fermi function, Fermi energy, free electron model and density of states, chemical potential of conduction electrons.
Module V: Non-equilibrium thermodynamics (10 lectures)
Thermodynamic criteria for non-equilibrium state, Phenomenological laws and Onsager reciprocal relations, Conservation of mass and energy in closed and open system. Entropy production: Due to heat flow, involving chemical reactions. Entropy production and entropy flow in open system. Transformation properties of fluxes and forces. Electrokinetic phenomena. Stationary non-equilibrium state: Prigogine's principle. Irreversible thermodynamics for biological systems.
Text books:
1. D. A. McQuarrie and J. D. Simon, Molecular Thermodynamics, Viva Books Private Limited, 1st Indian edition, 2004.
2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva, 1998.
3. C. Kalidas and M. V. Sangaranarayan, Non-Equilibrium Thermodynamics: Principles and Applications, McMillan India Ltd., 2002.
4. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics, Vikas Publishing House Pvt. Ltd., 6th ed., 2000.
5. S. Glasstone, Thermodynamics for Chemists, East-West Press Pvt. Ltd. 2008.

Reference books:
1. P. W. Atkins, Physical Chemistry, 7thed., Oxford University Press, New York, 2002.
2. I. N. Levine, Physical Chemistry, 5th ed., Tata McGraw Hill Pub. Co. Ltd., New Delhi. 2002.
3. F. W. Sears & G. L. Salinger, Thermodynamics, Kinetic Theory & Statistical Thermodynamics, Narosa, 1986.
4. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes. 3rded., Interscience, New York, 1978.

Course code: CH412
Course title: Analytical Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Module I: Introduction to Analytical Chemistry (10 lectures)

Types of analysis-qualitative and quantitative. Statistical analysis and validation: Errors in chemical analysis. Classification of errors- systematic and random, additive and proportional, absolute and relative. Accuracy and precision. Mean, median, average deviation and standard deviation. Significant figures and rules to determine significant figures. Calculations involving significant figures. Confidence limit, correlation coefficient and regression analysis. Comparison of methods: F-test and T-test. Rejection of data based on Q test. Least squares method for deriving calibration graph. Validation of newly developed analytical method. Certified reference materials (CRMs). Numerical problems.

Module II: Separation Techniques (10 lectures)

Chromatography: Definition and Classification. Techniques used in Paper, Thin Layer and Column chromatography. Applications in qualitative and quantitative analysis.

Ion exchange: Principle and technique. Types of ion exchangers. Ion exchange equilibria. Ion exchange capacity. Effect of complexing ions. Zeolites as ion-exchangers. Applications.

*Solvent extraction:*Principle and techniques. Distribution ratio and distribution coefficient. Factors affecting extraction efficiency: Ion association complexes, chelation, synergistic extraction, pH. Numericals based on multiple extractions. Role of chelating ligands, crown ethers, calixarenes and cryptands in solvent extraction. Introduction to Solid phase extraction (SPE) and Microwave assisted extraction (MAE), Applications.

Module III: Classical Methods of Analysis (9 lectures)

Volumetric analysis: General principle. Theory of indicators. Types of titrations with examples- Acid-base, precipitation, redox and complexometric. Titration curves for monoprotic and polyprotic acids and bases. Indicators used in various types of titrations. Masking and demasking agents.

Gravimetric analysis:General principles and conditions of precipitation. Concepts of solubility, solubility product and precipitation equilibria. Steps involved in gravimetric analysis. Purity of precipitate: Co-precipitation and post-precipitation. Fractional precipitation. Precipitation from homogeneous solution. Particle size, crystal growth, colloidal state, aging and peptization phenomena. Ignition of precipitates.

Module IV: Thermal Methods of Analysis (7 lectures)

Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis; thermometric titrations

Module V: Electrochemical Methods of Analysis (9 lectures)

Conductometry: Concepts of electrical resistance, conductance, resistivity and conductivity. Specific, molar and equivalent conductance and effect of dilution on them. Measurement of conductance. Kohlrausch's law, Applications of conductometry in determination of dissociation constant, solubility product. Conductometric titrations. High frequency titrations. Numerical problems.

Potentiometry: Circuit diagram of simple potentiometer. Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode and glass electrode. Reference electrodes: Calomel electrode and Ag/AgCl electrode. Theory of potentiometric titrations. Acid-base, redox, precipitation and complexometric titrations. Nernst equation, standard electrode potential, Determination of cell potential, n, K_f and K_{sp}. pH titrations. Buffers and buffer capacity. pH of buffer mixtures based on Henderson-Hasselbalch equation.

Text books:

1. G. D Christian, Analytical Chemistry. 5th ed., John – Wiley and Sons Inc., 1994.
2. D. A. Skoog, D. M. West and F. J. Holler, Fundamentals of Analytical Chemistry. 7th ed., Saunders College Publishing, 1996.
3. H. H. Willard, L. L. Merrit, J. A. Dean and F. A. Set, Instrumental methods of Analysis, CBS Publishers, 1996.

Reference books:

1. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5th ed., McGraw-Hill, New York, 1988.
2. A. J. Bard & L. R. Faulkner, Electrochemical methods, 2nd ed., Wiley, New York, 2000.
3. Vogel's text book of Quantitative Chemical analysis 5th edition, Ed., Jeffery et al. ELBS/Longman, 1989.
4. Encyclopedia of Analytical Chemistry: Ed. by R.A. Meyers Vol. 1-15, John Wiley, 2000.
5. D. M. Skoog, D. M. West and F. J. Holler, Fundamentals of Instrumental Analysis, 8th ed., Saunders College Publishing.

Course code: CH413
Course title: Inorganic Chemistry-V Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: T: P: 4
Class schedule per week: 04
Class: M.Sc. and I M.Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Syllabus

1. Semi micro qualitative analysis of mixtures containing two anions, two common cations and one rare earth elements: W, Mo, Ce, Th, Zr, V, U and Li.
2. Gravimetric determination of Fe in iron ore as Fe_2O_3.
3. Chemical Analysis of Alloy samples: Dissolution, sample preparation & Analysis. (any one)

a) Analysis of brass: Estimation of copper by gravimetry and zinc by EDTA titration.
b) Analysis of bronze: Estimation of copper by volumetry and tin by gravimetry

4. Inorganic Synthesis:

a) Nano-chemistry: Synthesis and characterization of manganese dioxide nanoparticles
b) Synthesis of pentaamminechlorocobalt(III) chloride.
c) Preparation of *cis* and *trans*-dichlorobis-(ethylenediamine)cobalt(III) chloride
d) Ligand synthesis for multimetal complex: Preparation of *bis*-(*N,N*-disalicylidene ethylenediamine)
e) Synthesis and characterization of *tris*-triphenylphosphinecopper(I) nitrate
f) Preparation of *bis*-(N, N'-disalicylalethylene-diamine)-μ-aquadicobalt(II)

Reference Books:

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS, 1986.
2. Vogel's text book of Quantitative Chemical Analysis, 5thEdition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical, 1999.
3. J. D. Woollins, Inorganic Experiments; VCH, Weinheim, 1994.

Course code: CH414
Course title: Theoretical & Computational Chemistry Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 **L:** 0 **T:** 0 **P:** 4
Class schedule per week: 04
Class: M.Sc. and I. M. Sc.
Semester / Level: M. Sc. II/ I. M. Sc. VIII
Branch: Chemistry
Name of Teacher:

Syllabus

1. A) Draw and clean the 2D chemical structure for given molecules (e.g.; Barbituric Acid,N-acetylneuraminic acid, Cholesterol) as per ACS format using ChemDraw Software. B) Perform the analysis of the drawn structure to report IUPAC name, molecular weight, exact mass and elemental analysis. C) Convert the 2D chemical structure into 3D structure using Chem3D software and demonstrate the various molecular models.
2. Draw the suitable conformers of 2,3-dibromobutane and demonstrate in Sawhorse, Newmann, and Fisher projection. Minimize the eclipsed and staggered conformor and evaluate the energies by molecular mechanics (MM) for both conformers.
3. Compute the physico-chemical properties such as log p, solubility, molar refractivity and NMR for a given molecule.
4. Draw the reaction mechanism for a given name reaction using ChemDraw tools in ACS (American Chemical Society) format.
5. Compute the partial atomic charges (extended Huckel) in phenol and display by color gradient.
6. Draw and demonstrate the HOMO-LUMO diagram using ethylene molecule. Minimize the energy of the given molecule and calculate HUMO-LUMO energy gap using Gaussian Software.
7. (a) Introduction about the computational chemistry software Schrodinger, understanding and use of its Graphical interface “Maestro” to prepare the molecular system for computer simulation. (b) Draw the 3D structure of a given chiral molecule (tamiflu) in Maestro workspace, clean the structure by short minimization using MM.
8. Generate the all stereochemical structure of a given molecules (tamiflu or zanamavir) using maestro interface of Schrodinger.
9. Conduct the molecular docking experiment for a given ligands with a large protein structure. Report the docking score and binding mode of ligands within the protein active site. Compare the docking result to conclude the remarks for its bindingaffinity.
10. Determine the single point energy of benzene (assume: singlet and uncharged) by density-function calculation with the B3LYP functional and a 6-31G** basis set. Optimize the geometry of the output structure form experiment-9 using BLYP/6-31G** level.
11. Run the calculation to demonstrate the electrostatic potential (ESP) of vinyl alcohol. Label atoms in the workspace with atomic properties derived from the ESP and examine the electrostatic potential (ESP) on the molecular surface.
12. Predict and describe the pKa values of organic bases such as methylamine, dimethyl amine and trimethyl amine usingChemOffice.
13. Draw and describe the 3D conformational features of *trans*-1,3-demthyl cyclohexane. Draw, demonstrate and compare the electrostatic potential map of CH_3-Cl and CH_3-Li. Explain the significance of this experiment.

Text books:

1. F. Jensen, Introduction to Computational Chemistry, Wiley, New York, 1999.
2. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory, 1st ed., revised Dover, 1989. More mathematical detail for many of the ab initio electronic structure methods.

Reference book:

1. D. A. McQuarrie, Quantum Chemistry, University Science Books, Mill Valley, CA, 1983.

Course code: CH501
Course title: Spectroscopic Elucidation of Molecular Structure
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

UV-Visible & IR Spectroscopy (8 Lectures)

Electronic transitions, Chromophores, Auxochromes, Bathochromic and hypsochromic shifts, Solvent effects, Woodward –Fieser Rules for dienes. enones and aromatic compounds.

Vibrational Transitions, Important group frequencies, Factors affecting I.R. group frequency, Applications of I.R. Instrumentation and recording of spectra.

Nuclear Magnetic Resonance Spectroscopy (10 Lectures)

1H-NMR: chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation for protons bonded to carbons and other nucleus, chemical exchange, effect of deuteration, complex spin-spin interaction between 2, 3, 4 and 5 nuclei, virtual coupling, stereochemistry, hindered rotation, simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects, 13C-NMR: General considerations, chemical shifts, coupling constants and examples 2D-NMR: spectroscopy-COSY, NOESY, DEPT. DEPT with 3 different angles, interpretation of 2D spectra and examples.

Mass Spectrometry (9 Lectures)

Introduction, ion production, factors affecting fragmentation, ion analysis, ion abundance, mass spectro fragmentation in organic compounds, common functional groups, molecular ion peak, high resolution mass spectrometry, examples of mass spectral fragmentation of organic compounds w.r.t. their structure determination.

Electron Spin Resonance Spectroscopy & Mossbauer Spectroscopy (11 Lectures)

Hyperfine coupling, Spin polarization for atoms and transition metal ions, spin orbit coupling an significance of g-tensors, applications to transition metal complexes having one unpaired electron including biological systems and to inorganic free radicals such as PH_4, F_2^- and $(BH_3)^-$.

Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display, applications to the study of bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds– nature of M-L bond, Co-ordination number, structure and detection of oxidation state.

Spectra and Structure: Combined application (7 Lectures)

UV, IR, NMR and Mass spectral data to elucidate unknown compound structure.

Text books:

1. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, McGraw-Hill Education; 6th ed. 2007.
2. R. M. Silverstein, F. X.Webster, D. J. Kiemle, Spectrometric Identification of Organic Compounds, 7th ed.; Wiley: Hoboken, NJ, 2005.
3. W. Kemp, Organic Spectroscopy, McMillan, Reprint 2009.

Reference books:

1. J. R. Dyer, Applications of Spectroscopy of Organic Compounds, Prentice Hall, Reprint 2010.
2. R. S. Macomber, A Complete Introduction to Modern NMR Spectroscopy, Wiley-Interscience; 1st ed., 1997.
3. H. Gunther, NMR Spectroscopy, Basic Principles, Concepts and Applications in Chemistry, 3rd ed., Wiley VCH, 2013.

Course code: CH 502R1 (SPL-I)
Course title: Inorganic Chemistry-VIII: Solid state and Nuclear Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I: Nuclear Structure and Stability (9 Lectures)
Nuclear Potential, Binding energy, empirical mass equation, The Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.

Module II: Nuclear reactions (9 Lectures)
Introduction, production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions. Fission and Fusion reactions: Fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and Asymmetric fission, decay chains and delayed neutrons.

Module III: The Structure of solids-I (12 Lectures)
The types of matter, classification of solids, close packing of atoms; Voids in closest packings; Radius ratio rule, Structure of ionic Crystals; Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX_2, spinel structure, perovskite structure. Perfect and Imperfect Crystals, intrinsic and extrinsic defects- Point defects, line and plane defects, Vacancies- Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defects formation, Colour centres, Non-stoichiometry and defects. Evolution of band structure, Brillouin zone, Effective mass of electron,

Module IV: The Structure of solids-II (7 Lectures)
Intrinsic semiconductors, Hall effect, Electrical conductivity of metals, alloys & semiconductors. Fermi levels in metals & semiconductors, Direct & indirect band gap semiconductors, Photo-conductivity, Properties of junctions: metal – metal, metal – semiconductor & semiconductor – semiconductor. Application: Diode system, Photocatalytic systems

Module V: Solid State Reactions (9 Lectures)
Thermal decomposition reactions- Type I, Type II, Polymorphism, Enantiotropy & Monotropy, Order-disorder transitions, Buerger's Classification, Polytypism, Sintering, Zone refining, Crystal growth, Growth from solutions, Flame fusion method, Vapour deposition technique, Chemical transport reaction, Growth by condensation.

Text books:

1. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th ed. Wiley Eastern, 1987.
2. A. R. West, Solid State Chemistry and its Applications, 2nd ed., Student Edition, Wiley, 2014.

Reference books:

1. G. Friedlander, T. W. Kennedy, E. S.Macias and J. M. Miller, Introduction of Nuclear and Radiochemistry, 3rd ed., John Wiley, 1981.
2. H. J. M. Bowen, Chemical Applications of Radioisotopes, Methuen, 1969.
3. C. N. R. Rao, New Directions in Solid State Chemistry, 2nd ed., Cambridge University Press, 1997.

Course code: CH503(SPL-I)
Course title: Molecular Spectroscopy
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I: Rotational spectroscopy (9 lectures)
Classification of polyatomic molecules: Linear, symmetric rotor, spherical rotor and asymmetric rotor molecules. The Stark effect in hetero-nuclear diatomic molecules. Rotational Raman spectroscopy. Applications of microwave spectroscopy.

Module II: Vibrational spectroscopy (9 lectures)
Infrared (IR) spectroscopy, Raman spectroscopy; Polyatomic molecules: Group vibrations, Number of normal vibrations of each symmetry species, Vibrational selection rules, Vibration-rotation spectroscopy, Anharmonicity. Techniques and instrumentation-Analysis by IR spectroscopy.

Module III: Electronic spectroscopy (9 lectures)
Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Transition moments, assignment of electronic transitions of N_2, H_2O and formaldehyde using group theory. Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding. Fluorescence and phosphorescence.

Module IV: Photoelectron spectroscopy (9 lectures)
Ionization processes and Koopman's theorem, Ultraviolet photoelectron spectroscopy, X-ray photoelectron spectroscopy. Auger electron spectroscopy: introduction- instrumentation- classification of various transitions- quantification- applications**.** Electron energy loss spectroscopy: Franck and Hertz experiment- instrumentation - selection rules- theory- studies on molecules- surface states- high resolution spectroscopy- adsorption and catalysis- applications.

Module V: Spin resonance spectroscopy (9 lectures)
The effect of magnetic fields on electron and nuclei, nuclear magnetic resonance (NMR): Bloch equations, Steady state (continuous wave) and Transient (pulsed) experiments, nuclear Overhauser effect, Polarization transfer, Selective Population Inversion. Electron spin resonance (ESR): g value, hyperfine structure, ESR of organic free radicals, solids, inorganic ions, simple free radicals in solutions. Mossbauer spectroscopy: principle & applications.

Text books:

1. P. W. Atkins, J.de Paula, Physical Chemistry, Oxford, London, 7th ed. 2002.
2. P. S. Sindhu, Fundamentals of Molecular Spectroscopy, New Age International (P) Ltd. Publishers, 2006.
3. C. M. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
4. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.
5. M. Hollas, Modern Spectroscopy, Wiley; 4th ed., 2004.

Reference books:

1. A. Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Methuen, 1983.
2. J. D. Graybeal, Molecular Spectroscopy, McGraw Hill, 1993.
3. H. Friebolin, Basic One- and Two-Dimensional NMR Spectroscopy 5th ed., Wiley-VCH, 2010.

Course code: CH504R1 (SPL-I)
Course title: Advanced Organic Synthesis
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I: Hydroboration reactions (10 Lectures)
Introduction, synthetic application of organobroranes: isomerization, formation of C-C bonds, aldehydes, ketones, trialkylcarbinols, reactions of alkenylboranes and trialkylalkynyl borates, free-radical reactions of organoborane.

Module II: Reagents for Oxidation (10 Lectures)
SeO_2, CrO_3, CrO_2Cl_2, LTA, t-BuOOH, mCPBA, $PdCl_2$, $HgSO_4$, $KMnO_4$, OsO_4, OsO_4/RuO_4, H_2O_2, $C_6H_5CO_3H$, CF_3CO_3H, I_2/Py, HIO_4, PCC, PDC, Des-Martin periodinane, IBX, NBS, $AgNO_3$, Ag_2CO_3, Ag_2O, AgO, MnO_2, $NaIO_4$ cat. Ozone, DDQ, DDQ/PbO_2.

Module III: Reduction (10 Lectures)
Catalytic hydrogenation and hydrogenolysis of various functional groups by Pt_2O, Pd/C, raney nickel, Homogeneous hydrogenation by transition metal complexes {Rh, Ru}, dissolving metal {Li, Na in Liq. NH_3, Zn/HCl or CH_3COOH}, non-metallic reducing agent {hydrazine, Et_3SiH, Ph_2SiH_2, formic acid}, Metal hydrides-based Reduction: $LiAlH_4$, alkoxyaluminate, DIBAL-H, $NaBH_4$, $NaBH_3CN$, $LiBH_4$, $Zn(BH_4)_2$, $NaBH_4/CeCl_3$, alkoxy/alkyl borohydrides, super-hydride, selectrides, n-Bu_3SnH

Module IV: Retrosynthetic analysis (10 Lectures)
1,3-difunctionalised compounds, α, β-unsaturated carbonyl compounds, control in carbonyl condensation, 1,5-difunctionalised compounds. Michael addition and Robinson annelation, Retrosynthetic analysis and synthetic design of Tamiflu and Reserpine.

Module V: frontier in organic chemistry (10 lectures)
Chemical and drug industry, examples, environmental issues, green synthetic technique, examples, research orientation of chemistry, emerging field in chemistry, recent development of chemistry.

Text books:

1. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 2nd ed., Oxford Press, 2012.
2. I. L. Finar, Organic Chemistry, Vol. I & II, 5th ed., Longman Ltd., New Delhi, 2011.
3. R. S. Monson, Advanced Organic Synthesis, Academic Press, New York, 2012.

Reference books:

1. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th ed., 7th Indian Reprint, Pearson Education, 2005.
2. Jerry March, Advanced Organic Chemistry, Wiley, 7th ed., 2013
3. Carey and Sundberg, Advanced Organic Chemistry, Springer, 5th ed.; 2000

Course code: CH 505 (SPL-II)
Course title: Inorganic Chemistry-IX: Bio Inorganic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I Basic Bio-inorganic Chemistry (9 Lectures)
Elements of life, the natural selection of elements, metallo-biomolecules– enzymes and proteins, their differences, Metal ion storage and transport: Ferritin, metallothioneins, cerruloplasmin; Siderophores– enterobactin, transferin;. Na^+, K^+ pump, Ca^{2+} transport.

Module II Oxygen management and oxygen transport (9 Lectures)
Kinetics of biological and non-biological oxygenation, Reactive Oxygen Species (ROS): Occurance, types, active site structure and mechanism Super oxide dismutase , Catalase, Peroxidase.
Natural Oxygen carriers: Heme Type: Myoglobins and Hemoglobins, Properties of heme and iron-porphyrins, The heme iron–dioxygen bond, Mechanism of dioxygen binding and model systems. Di-iron Type: Hemerythrins and Myohemerythrins : Early history and distribution of hemerythrins, Protein structure , The di-iron site and formulation of the O_2 binding reaction, Mechanism of dioxygen binding, Autoxidation, Cooperative hemerythrins, Dicopper Type: Hemocyanins: Protein structure and superstructure, The dicopper site, Mechanism of dioxygen binding.

Module III Hydrolase and Oxido-Reductase Enzymes (9 Lectures)
Zn Carbonic Anhydrase, Zn Carboxy peptidase, Fe Acid Phosphatase, Ni Urease, Alcohol dehydrogenase-Occurance, types, active site structure and mechanism and model system. catalytic activity of Cu proteins for biological oxidation: Tyrosinase, Galactose oxidase, Catecholase, phenoxazinone synthase.

Module IV Model Systems in Bioinorganic Chemistry (9 Lectures)
Chemistry of Vitamin B_{12} , Iron– Sulphur proteins, Cytochrome c Oxidase, Cytochrome P– 450, Nitrogenase- biological nitrogen fixation, molybdenum nitrogenase, Nitrogenase model systems, Hydrogenase and model systems, Metal complexes in transmission of energy- Chlorophylls & Photosynthetic Water Oxidation.

Module V Metals in Medicine (9 Lectures)
Metal Toxicity and Homeostasis, Chelation Therapy, Vanadium-Based Diabetes Drugs, Pt based Anti-Cancer Drugs, Mechanism of cisDDP Antitumor Activity, Anti-arthritis drugs, Imaging Agents: Technetium Imaging Agents, Gadolinium MRI Imaging Agents, Gold containing drugs used in the therapy of Rheumatoid Arthritis, Lithium in psychopharmalogical drugs.

Text books:

1. I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valentine,Bioinorganic Chemistry, University Science Books, Mill Valley, CA, 1994.
2. W. Kaim, B. Schwederski, A. Klein, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: An Introduction and Guide, Wiley, 1994.
3. L. Stryer, J. M. Berg, J. L. Tymoczko, 5th ed.,W. H. Freeman & Co Ltd, 2002.

Reference books:

1. R. R. Crichton, Biological Inorganic Chemistry, 2nd ed., Elsvier, 2012.
2. R. M. Roat-Malone, Bioinorganic Chemistry: A Short Course, Wiley, 2002.

Course code: CH506 (SPL-II)
Course title: Advanced Electrochemistry
Pre-requisite(s): B.Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I: Electrode Kinetics (9 lectures)

Mass transfer by Diffusion and Migration – models of electrode reactions – current potential characteristics–general mass transfer equation. Kinetics of an electrode reaction, Butler-Volmer equation, diffusion overpotential. Exchange current density, Tafel plot. Polarizable and non-polarizable interfaces. Irreversible electrode processes.

Module II: Corrosion (9 lectures)

Different types of corrosion; Evans diagram, Pourbaix diagram; Corrosion current and Corrosion potential; Measurement of corrosion rate; Stern Geary equation; Mixed potential theory and prevention of corrosion.

Module III: Electroanalytical Techniques (10 lectures)

Potential Step Methods: Types of techniques, step under diffusion control, Ilkovic equation– polarographic analysis–sampled current voltammetry, reversible, irreversible processes, multicomponent systems. *Chrono Methods:* Chronoamperometry, chronocoulometry. *Pulse polarographic methods*; *Potential Sweep Methods:* Cyclic Voltammetry; *Bulk Electrolysis Techniques:* Classification of methods–Controlled Potential methods: current – time behaviour, electrogravimetry, electroseparation–Coulometric measurements: controlled current methods: characteristics, coulometric methods–Electrometric end point detection: classification, potentiometric, amperometric methods.

Module IV: Spectro-electrochemical and spectroscopic techniques (7 lectures)

Impedance Spectroscopy, Scanning Electrochemical Microscopy, Electrochemical AFM and STM, Electrochemical Quartz Crystal Microbalance.

Module V: Electrochemical Energy Systems (10 lectures)

Electrochemical power sources - theoretical background on the basis of thermodynamic and kinetic considerations. Primary cells, secondary cells- magnesium and aluminium based cells magnesium reserve batteries, Li-ion batteries. Fuel cells - classification - chemistry of fuel cells - detailed description of hydrogen/oxygen fuel cells - methanol - molten carbonate solid polymer electrolyte and biochemical fuel cells. Photoelectrochemical cells, Electrochemical supercapacitors for energy storage.

Text books:

1. J.O'M. Bockris & A. K. N. Reddy, Modern Electrochemistry, Vol. 1 & 2A and 2 B, Plenum Press, New York, 2000.
2. A. J. Bard and L. R. Faulkner, Electrochemical methods, Wiley & Sons, 2nd ed., 2001.
3. S. Glasstone, Introduction to Electrochemistry, East West Press, reprint 2007.

Reference books:

1. D. R. Crow, The Principle of electrochemistry, Chapman Hall, 4th ed. 1994.
2. H. Kissinger, Electroanalytical Techniques, John wiley, 1998.
3. P. H. Reiger, Electrochemistry, Prientice Hall, 1987.

Course code: CH 507R1 (SPL-II)
Course title: Selected Topics in Organic Synthesis
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T:1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Module I: Conformation and Reactivity [10 Lectures]
Conformation around sp^3-sp^2 and sp^2-sp^2 bond, conformation around carbon hetero atom bond, conformation of cyclohexane with 1/2 sp^2 bond, conformation analysis of heterocycles, reactivity in cyclohexane with 1/2 sp^2 bond cyclic system (substitution, addition, elimination, rearrangement etc.).

Module II: Stereochemistry [10Lectures]
Optical rotatory dispersion (ORD) and circular dichroism (CD), classification of ORD and CD Curves, Cotton effect curves and their application to stereochemical problems; the Octant rule and its application to alicyclic ketones, in absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, geometrical isomerism in alkenes and oximes, methods of determining the configuration.

Module III: Advanced Stereochemistry (10 Lectures)
Optical isomerism in compounds without any stereocenters (allenes, biphenyls), Enantiomerism in allenes, alkylidene cycloalkane, spiranes- configurational nomencalture, correlation of axial dissymmtry and centrodissymmetry, Stereochemistry of natural products, strychnine, podophyllotixin, Conformation and reactivity of fused polycyclic systems: perhydrophenanthrenes.

Module IV: Pericyclic Reaction (8 Lectures)
2+2 addition of ketenes, 1,3 dipolar cycloadditions and Cheleotropic Reactions, Effect of Diene and dienophile stereochemistry, Endo rule in Diels-Alder Reaction, Reverse electron Demand Diels-Alder Reaction, Intramolecular Diels-Alder Reaction, Regioselective Diels-Alder Reactions, Heterocyclic synthesis: Principles of heterocyclic synthesis involving cyclization and cycloaddition (1,3-dipolar, hetero-diels alder and 2+2 cycloaddition reactions). 3,3- and 5,5-sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements, Ene and Retro Ene Reactions.

Module V: Heterocyclic Chemistry (9 Lectures)
Synthesis, medicinal applications and reactions of oxirane, aziridine, azetidinone (β-lactam), oxetane, pyridine, pyrylium salts and pyrones. Heterocyclic chemistry of benzo-fused derivatives: Synthesis, medicinal applications and reactions of benzofurans, benzothiophenes, quinolines, isoquinolines, quinolizines, Indolizines, benzopyrylium salts, coumarin, chromene, chromones.

Text books:
1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications; New Age International Publishers, 2018
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanism and Structure, 7ed, Wiley, 2015.
3. W. Carruthers, I. Coldham, Some modern methods of Organic Synthesis, 4th ed., Cambridge Univ. Press, 2015.
4. S. Warren, Organic Synthesis: The Disconnection Approach, Wiley 2007

Reference books:
1. E. L. Eliel, Stereochemistry of Organic Compounds, Wilel, 2008
2. S. Warren, P. Wyatt Workbook for Organic Synthesis: The Disconnection Approach, 2nd ed., Wiley, 2010.
3. Norman and Coxon, Principle of Organic Synthesis, 3rd ed., CRC Press, 1993.
4. I. Ojima, Catalytic Asymmetric Synthesis, 3rd ed, John Wiley & Sons, New Jersey, 2010.
5. V. Sunjic, V. P. Perokovic; Organic Chemistry from Retrosynthesis to Asymmetric Synthesis, Springer, 2016

Course code: CH 508
Course title: Advanced Characterization Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Syllabus

I: Examples of organic sample characterization by UV-VIS, IR, NMR, Mass, CHN, mp and single crystal diffraction techniques.

Experiment 1: Synthesis and characterization of sugar intermediates using UV, IR, NMR (^{1}H and ^{13}C), Mass, mp and CHN.

Experiment 2: Synthesis of Nucleo-base analogs and characterization using UV, IR, NMR (^{1}H and ^{13}C), Mass, mp and CHN.

Experiment 3: Synthesis of Benzanilide and characterization using UV, IR, NMR (^{1}H and ^{13}C), Mass, mp and CHN.

II: Examples of bimolecular and polymeric materials characterization using Intense Viscosity Measurement, Molecular Weight Determination and Distribution using GPC, Light Scattering Technique, FTIR, NMR, SEM, XRD

Experiment 1: Determination of T_g and T_m of Polyvinyl chloride and methylmethacrylate polymer using TGA/DSC.

Experiment 2: Study of surface morphology of polymeric material /hybrid materials using XRD and SEM.

Experiment 3: Finding out molecular weight of PMMA using light-scattering/GPC.

III: Examples of inorganic sample characterization

Experiment 1: Thermogravimetric analysis of $CuSO_4.\ 5H_2O$

Experiment 2: Synthesis & characterization of Fluorescent Zn complexes by spectrofluoremeter.

Experiment 3: Study of surface morphology of inorganic materials using XRD and SEM.

Reference book:

1. V. R. Gowariker, N. V. Viswanathan & J. Sreedhar, Polymer Science, New Age International (P) Ltd. Publishers, 1986.
2. W. Kemp, Organic Spectroscopy, Palgrave, Reprint 2009.
3. Suryanarayana, C.; Norton, M. G. X-Ray Diffraction - A Practical Approach, Springer Publishers, 1998.
4. Lyman, C. E. et al., K.-R.Scanning Electron Microscopy, X-Ray Microanalysis, and Analytical Electron Microscopy, Springer Publishers, 1990.

Course code: CH 509
Course title: Inorganic Chemistry (SPL) Lab
Pre-requisite(s): B.Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: T: P: 4
Class schedule per week: 04
Class: M.sc. and I M.Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Syllabus

1. Determination of conductivity of 1:1, 1:2 and 1:3 complexes.
2. Kinetics of Hg(II) catalysed reaction of $[FeCN_6]^{4-}$ with 1,10-*ortho* phenonthroline and its application in the determination of trace quantity of Hg(II).
3. Study of the conductance of $H[Co(DMGH)_2Cl_2]$ in freshly prepared aqueous solution and its change with time for studying the rate of aquation.
4. pH metric determination of Proton- Ligand and Metal-Ligand stability constants.
5. Colorimetric study of the kinetics of the reduction of azidopentaminecobalt(III) chloride by aqueous Fe(II) ion.
6. Colorimetry: Simultaneous determination of chromium and manganese in a solution by visible spectroscopy.
7. Spectrofluorometric determination of lanthanide elements in dilute solution.
8. Quantitative determination of DNA–Ligand binding using fluorescence spectroscopy.
9. Determination of magnetic moment of the lanthanides by Gouy's method.
10. Use of ligand field tetragonality on the ground state spin of Ni(II) complexes.
11. Determination of formal potential of electronically non-innocent ligands.
12. Determination of formal potential of metal complexes.

Reference books:

1. M. V. Cases, Principles of analytical chemistry, Springer, 2000.
2. D. Harvey, Modern Analytical Chemistry; Mcgraw-Hill, 2000.
3. A. J. Bard and I. Rubinstein, Electroanalytical Chemistry, CRC Press, 1998.
4. Electroanalytical Chemistry: A Series of Advances: Volume 24, A. J. Bard and C. Zoski, CRC Press, 2017.

Course code: CH 510
Course title: Physical Chemistry (SPL) Lab
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Syllabus

1. To determine pH of a buffer solution using quinhydrone electrode.
2. Oscillatory reaction: Chemical oscillation & pattern formation in B-Z system.
3. To study the phase diagram of two components forming a simple eutectic.
4. To determine the molecular weight of a polymer from viscosity measurements.
5. To determine magnetic susceptibility by Guoy balance.
6. To determine the surface area of alumina by BET surface area determination method.
7. To determine the solubility product by conductivity and potentiometric methods.
8. Stability constants of complexes by the use of pH meter, potentiometric method.
9. Reversibility of an electrochemical reactions and determination of concentration of a given reducible ion-Polarography.
10. To determine the Tafel constants, the corrosion current and the linear polarisation resistance from polarisation curves.
11. Electrochemical impedance spectroscopy (EIS) study and formation of equivalent circuit diagram.
12. To determine the effect of change of temperature, concentration of reactant and catalyst and ionic strength of the media on the velocity constant of hydrolysis of an ester.

Text books:

1. B. Viswanathan, and P. S. Raghavan, Practical Physical Chemistry, Viva Books, 2010.
2. J. B. Yadav, Advanced Practical Physical Chemistry, 22nd edition, Goel publishing House, Krishna Prakashan Media Ltd. 2005.
3. V. Venkatesan, R. Veeraswamy and A.R. Kulandaivelu, Basic Principles of Practical Chemistry, 2nd ed., Sultan Chand and Sons Publication, New Delhi. 1997.
4. D. Harvey, Modern Analytical Chemistry; Mcgraw-Hill, 2000.

Reference books:

1. B. P. Levitt, Findlays Practical Physical Chemistry, 9th ed., Longman, London, 1985.
2. G. R. Chatwal and S. K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publishing House, Delhi, 2000.
3. A. M. Halpern and G. C. McBane, Experimental Physical Chemistry: A Laboratory Text Book, 3rd ed., W. H. Freeman, 2006.

Course code: CH 511
Course title: Organic Chemistry (SPL) Lab
Pre-requisite(s): B.Sc. (H) Chemistry
Co- requisite(s):
Credits:2 L: 0 T: 0 P: 4
Class schedule per week: 04
Class: M.Sc. and I. M. Sc.
Semester / Level: M. Sc. III/ I. M. Sc. IX
Branch: Chemistry
Name of Teacher:

Syllabus

1. Synthesis of alcohol from the reaction of a Grignard reagent and a ketone.
2. Synthesis of an alkene from dehydration of the alcohol prepared in previous step.
3. Multi-step reactions, (Cyclohexanone to methyl cyclohexane) using i) Grignard reaction ii) Dehydration iii) High-pressure hydrogenation.
4. Anthranilic acid from phthalic anhydride.
5. Synthesis of Nylon 6 starting from cyclohexanone.
6. Characterization of an organic compound through CHN, Mass, FTIR, NMR and single crystal X-ray diffraction.

Reference Books:

1. A. I. Vogel, Quantitative Organic Analysis, Part 3, Pearson, 2012.
2. F. G. Mann, & B. C. Saunders, Practical Organic Chemistry, Pearson Education, 2009.
3. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Practical Organic Chemistry, 5th ed., Pearson, 2012.
4. V. K. Ahluwalia and R. Aggarwal, Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press, 2000.
5. V. K. Ahluwalia and S. Dhingra, Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press, 2000.

Course code: CH 513 (SPL-III)
Course title: Inorganic Chemistry-X: Inorganic Photochemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. IV/ I. M. Sc. X
Branch: Chemistry
Name of Teacher:

Module I Photophysical properties of excited state (9 Lectures)
Absorption spectra and electronic transitions, Assignment of electronic transitions, Charge transfer transition, Radiative decay, Non-radiative decay and the energy gap law, Classification of the excited state- MLCT, MC & LC excited state, Reactivity pattern of the excited state, Electronic excited state of d^3 and d^6 complexes, Solvent effects and dipole moment of the excited state, Acid- base reactions of the excited states.

Module II Photochemical reactions and techniques for the study of excited state (9 Lectures)
Bimolecular quenching of the excited state, Energy and electron transfer quenching, Energetics, Photoredox reactions of metal complexes - Thermal electron transfer process: Classical treatment and self exchange type, Energy transfer reactions of the excited state, Excited state acid-base reactions, Photoinduced electron transfer, Photoinduced energy transfer (Forster and Dexter mechanism), Characterization of the excited state by steady state methods and Time-Resolved methods (Flash Photolysis), Time resolved conductivity, Electron spin resonance, Photoselection, Study photo-redox and energy transfer reactions, Study of the photosubstitution reactions.

Module III Photochemistry of the Polypyridyl complexes (9 Lectures)
Polypyridyl ligands as chelating agents, Free ligand and metal complexes excited state, Ground and excited state redox properties, General trends in polynuclear and ortho-metallated complexes, Polypyridyl complexes of Fe, Ru, Os, Cr and Cu Photochemical applications of Polypyridyl complexes: Catalysed photodecomposition of H_2O to H_2, and O_2, Catalysed photoreduction of CO and CO_2, $Ru(bpy)_3^{2+}$ as dye for DSSC.

Module IV Photochemistry of Porphyrins (9 Lectures)
Introduction to porphyrin, Classification of porphyrins, Electronic spectroscopy of metalloporphyrin, Classification based on absorption and emission spectral feature, Description on metalloporphyrin ground and excited state. Resonance Raman spectra of metalloporphyrins. Hypso porphyrins: luminiscent type- Cu and Ag Porphyrin, Phosporescent type- Au, Pt, Pd, Rh, Ru and Os Porphyrins; Radiationless Hypso Porphyrins: Fe and Co Porphyrins, Hyper porphyrine: d type- Cr and Mn Porphyrins, p Type-Metalloid porphyrins; Pseudo normal Porphyrins-Lanthanide porphyrins..

Module V Application of Inorganic Photochemistry (9 Lectures)
Environment cleaning: Photocatalytic reactions of volatile hydrocarbons, Photocatalytic activity of TiO_2 in cleaning air pollutants, Photocatalyst based air purifying materials.
Porphyrin and photosynthesis, Active site structure of Chlorophyl, Accessory Pigments and Extended Range of Light Absorption, Exciton Transfer; Central Photochemical Event: Light-Driven Electron Flow, The Pheophytin-Quinone Reaction Center, Functional modules of photosynthetic machinery- *Z* Scheme, Biomimetic energy production- Artificial photosynthesis, Photosynthetic cell, Dye Sensitised Solar Cell, Tandem Cell.

Text books:
1. K. Kalyanasundaram, Photochemistry of Polypyridine and Porphyrin Complexes; Academic Press Limited: London, 1992.

Reference books:
1. M. Kaneko, I. Okura, Photocatalysis: Science and Technilogy, Springer
2. E. A. B. Ebsworth, D. W. H. Rankin, S. Cardock, Structural methods in Inorganic Chemistry; 2nd ed., Wiley-Blackwell, 1991.

Course code: CH 514 (SPL-III)
Course title: Chemical Applications of Group Theory
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. IV/ I. M. Sc. X
Branch: Chemistry
Name of Teacher:

Module I: Molecular Vibrations (9 lectures)
Group theory and normal modes of vibrations of polyatomic molecules. Procedure for determining the irreducible representation of the vibrational modes for H_2O, NH_3 molecules. Selection rules for fundamental vibration transition.

Module II: Molecular Orbital (MO) Theory & its Application in Organic Chemistry (9 lectures)
Symmetry factoring of secular equations, carbocyclic system, LCAO-MO π-bonding for naphthalene & formaldehyde. Electronic excitation, Selection Rule and Configuration interaction, Three-centre bonding, Symmetry-based selection rule for cyclization reaction.

Module III: MO Theory for Inorganic & Organometallic Compounds (9 lectures)
Transform properties of atomic orbitals, hybridization scheme for σ & π bonding orbitals; MO theory for AB_n-type of molecules and regular octahedral and tetrahedral molecules.

Module IV: Ligand Field Theory (9 lectures)
Electronic structure of free atoms and ions; Splitting of levels and terms in chemical environment, Construction of energy level diagrams; Estimation of orbital energy; Selection rules and polarization; Double groups.

Module V: Crystallographic Symmetry (9 lectures)
Two-dimensional space symmetries; Three-dimensional and their symmetries; Crystal symmetry; Interrelating lattice symmetry, crystal symmetry & diffraction symmetry; Additional symmetry elements & operations; Space groups and X-ray crystallography.

Text books:

1. F. A. Cotton, Chemical Applications of Group Theory, 3rded., Wiley Eastern Limited, 1985.
2. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, 1986.

Reference books:

1. P. Atkins, R. Friedman, Molecular Quantum Mechanics, 4th ed., Oxford University Press, 2005.

Course code: CH 515 (SPL-III)
Course title: Interdisciplinary Organic Chemistry
Pre-requisite(s): B. Sc. (H) Chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: M. Sc. and I. M. Sc.
Semester / Level: M. Sc. IV/ I. M. Sc. X
Branch: Chemistry
Name of Teacher:

Module I: Carbohydrate chemistry (10 Lectures)

Biological importance of monosaccharides (aldohexose-glucose, mannose, galactose; epimers; ketohexose–fructose,; aldopentose-riboses; deoxysugars-deoxyribose; fucose; rhamanose), polysaccharides (cellulose, glycogen, starch, chitin, agar), Glycoprotein, proteoglycan, glycosaminoglycan, muramic acid, sialic acid. Molish's test for carbohydrate, reaction of monosaccharides with nitric acid, bromine water, periodic acid and phenylhydrazine, osazone formation, reaction of deoxyribose with DPA and reaction of ribose with orcinol reagent; glycosidic linkage, disaccharides (sucrose-invert sugar, inversion of sucrose, maltose and lactose) reducing and non-reducing sugar (tests for reducing sugars, reaction with Benedict's reagent, Fehling's solution, Tollen's reagent, Seliwanoff test for ketose)

Module II: Peptide Chemistry (10 Lectures)

Example of biologically important peptides and their functions in brief (glutathione-peptide of non-protein origin), Merrifield solid-phase peptide synthesis using protection/ deprotection protocol (brief outline). Deprotection and racemization in peptide synthesis. Solution and solid phase techniques. Proteins: Definition & structure, primary, secondary, tertiary and quaternary structure (definition and example), structure of globular protein (albumin, globulin, haemoglobin & myoglobin – Structure, function and occurrence in brief) Behaviour of proteins in solutions, salting in and salting out, Denaturation and renaturation of proteins (example -RNase), absorbance of proteins, example of metalloprotein, lipoprotein.

Module III: Natural Product Chemistry (9 Lectures)

Flavonoid Chemistry: Anthocyanims, Flavonols and flavones; Quinone chemistry. Terpenoids: Structure and Methods for Structure elucidation. Biosynthesis of Terpenoids: Gibberellins. Acyclic (Squalene), Lanosterol, Ursolic acid & Oleanolic acid. Alkaloid Chemistry: Opium, Ergot, Rauwolfia and Vinca alkaloids. Cyanogenic glycosides, Indoles and Chlorophylls. Steroid chemistry: Introduction & Biosynthesis of Steroids. Phytosterols, Saponins & Sapogenins, Cardiotonic glucosides, Steroidal alkaloids: Solanum and Kurchi alkaloids.

Module IV: Polymer Chemistry (8 Lectures)

Methods of polymerization: Bulk, solution, suspension, emulsion, Addition, Melt and condensation.
Properties of polymers: Viscosity, end-group analysis, hardness, abrasion resistance, crystallinity glassy state, glass transition temperature (T_g) and melting point (T_m).
Additives in polymers: Plasticizers, stabilizers, antioxidants, fillers, pigments
Polymer processing: Compounding, calendaring, die/rotational/film casting, injection molding, extrusion molding, thermoforming, foaming and reinforcing.

Module V: Green Chemistry (8 Lectures)

Introduction to the principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reduce derivatives, renewable feedstock, catalysis, design for degradation, Green synthesis, clean routes, supercritical solvents, ionic liquids, Catalysis in green chemistry.

Text books:

1. I. L. Finar Organic Chemistry Vol. II., Stereochemistry and the Chemistry Natural Products, 5th ed., Longman Ltd., New Delhi, 2011.
2. A. Ravve, Principles of Polymer Chemistry, Plenum Press, New York, Springer 3rd Edition, May 2012.
3. V. R Gowarikar, Vishwanathan Srikanth, Polymer Chemistry, Wiley Eastern, Bombay, 2000.
4. V. K. Ahluwalia, Green Chemistry: Greener Alternatives to Synthetic Organic Transformations- Narosa Publishing House.

Reference books:

1. T.K. Lindhorst: Essentials of Carbohydrate Chemistry and Biochemistry, 3rd ed., Wiley-VCH, Weinheim 2007.
2. P. D. Bailey, An Introduction to Peptide Chemistry; Wiley-Blackwell; Revised ed. edition (22 April 1992)
3. S. V. Bhat, B. A. Nagasampagi, M. Shivakumar: Chemistry of Natural Products; Narosa Publishing House; Revised edition (27 September 2013)
4. V. K. Ahluwalia, Anuradha Mishra Polymer Science:, Ane Books Pvt. Ltd.
5. M. Lancaster, Green Chemistry: In Introductory Text, RSC Publishing, 2010

BTECH PROGRAMME

(CH 101) Chemistry

Credits: 4 L: 3 T: 1 P: 0
Class: B. Tech.
Semester / Level: I

Module I: Chemical Bonding

Ionic bond: Radius ratio rule, Born-Landé equation, Born-Haber cycle. *Metallic Bond:* valence bond and band theories, defects in solids, Werner's Theory, Bonding in Transition metal complexes, Ligands, coordination complexes, Ligand Field, Crystal Field Theory, Octahedral, Tetrahedral and square planar complexes, CFSE, Jahn Teller theorem, electronic spectra, magnetism, and isomerization in coordination compounds. **[9L]**

Module II: Organic Structure and Stereochemistry

Covalent bond: Lewis structure, Valence Bond theory, Molecular orbital theory, Molecular orbital of diatomic and polyatomic system, hybridization, conjugated molecules, Huckel molecular orbital theory of conjugated systems. Isomerism, Geometrical isomerism: *cis–trans* and syn-anti isomerism; Optical isomerism & Chirality; Wedge, Fischer, Newmann and Sawhorse Projection formulae and interconversions; E/Z, D/L, R/S nomenclature system; Conformational studies of ethane, n-butane, Cyclohexane. **[9L]**

Module III: Kinetics and Catalysis:

Order & molecularity of reactions: chain, parallel, Competing, Side, Consecutive reactions; Kinetics of Fast reactions, Characteristics of catalyst, types of catalysis, catalytic poison; Theories of catalysis; Acid base catalysis: including kinetics, Enzyme catalysis, Mechanism and kinetics of enzyme catalyzed reaction, Michaelis-Menten equation, Important catalysts in industrial processes; Hydrogenation using Wilkinsons catalyst, Hydroformylation by using Cobalt-catalyst, Phase transfer catalyst. **[9L]**

Module-IV: Spectroscopic Techniques

Absorption and emission Spectroscopy, Lambert-Beers Law, Principles and applications of UV-Visible, Factors influencing for UV-VIS spectrum; Rotational and Vibrational spectroscopy, Principle of FT-IR, and NMR spectroscopy; Modern techniques in structural elucidation of compounds by UV-VIS, IR, & NMR Spectroscopy. **[9L]**

Module V: Phase and Chemical equilibrium

Phase Rule: Terms Involved, Phase diagram of one component (Water) & two component (Pb/Ag) system & their applications. Law of chemical equilibrium, equilibrium constants and their significance, Weak and strong electrolytes, Standard electrode potential and its application to different kinds of half cells, EMF and its measurement and application, Batteries and Fuel Cells, Chemical and Electrochemical corrosion, Factors affecting the rate of corrosion.

[9L]

Text books:

1. Huheey, J. E., Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, Pearson.
2. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Seventh Edition, Pearson
3. Atkins, P. W. & Paula, J. Physical Chemistry, 10th Ed., Oxford University Press, 2014.

Reference books:

1. Lee, J. D. Concise Inorganic Chemistry ELBS, 1991.
2. Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier (2009).
3. William Kemp, Organic Spectroscopy, 3rd Ed., 2008 Macmillan.

Course code: CH 102
Course title: Chemistry Lab
Pre-requisite(s): Intermediate level Chemistry
Co- requisite(s):
Credits: 1.5 L: 0 T: 0 P: 3
Class schedule per week: 03
Class: B. Tech.
Semester / Level: I
Branch: Chemistry
Name of Teacher:

Syllabus

1. Gravimetric estimation of Nickel by Dimethylglyoxime.
2. Quantitative estimation of Ca^{2+} and Mg^{2+} ions by complexometric titration using Na_2-EDTA.
3. To verify Bears Law using Fe^{3+} solution by spectrophotometer/colorimeter and to determine the concentration of a given unknown Fe^{3+} solution.
4. Separation of binary organic mixture by acid-base extraction and analysis using given FTIR and NMR spectrum.
5. Preparation of Diazoamino Benzene and report the melting point and yield of product.
6. Draw melting point-mass percent composition diagram for two component mixture and determine the Eutectic Temperature.
7. To study the kinetics of acid-catalyzed hydrolysis of ethyl acetate and to evaluate the value of the rate constant.
8. To determine the rate law for the reaction between iodide and hydrogen peroxide in an acidic environment and to determine the effect of a catalyst on the rate of reaction.
9. To determine the strength of the given strong acid by strong base Potentiometrically.
10. To determine the transition temperature of the given salt hydrate.
11. Qualitative detection of special elements in organic compounds.
12. To draw the pH-titration curve of strong acid vs strong base.

Reference book:

1. Experimental Physical Chemistry, By B. Viswanathan, P. S. Raghavan, Narosa Publishing House (1997).
2. Vogels Textbook of Practical Organic Chemistry
3. Experiments in General chemistry, C. N. R. Rao and U. C. Agarwal
4. Experimental Organic Chemistry Vol 1 and 2, P R Singh, D S gupta, K S Bajpai, Tata McGraw Hill

FOUNDATION SCIENCE (FS) FOR IMSc PROGRAMME

Course code: CH 111
Course title: General Chemistry-I
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: B. Sc.
Level: I
Branch: Chemistry
Name of Teacher:

Module I: Atomic Structure (9 Lectures)
Bohr's theory, Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule, Aufbau's principle, Variation of orbital energy with atomic number.

Module II: Periodicity of Elements (9 Lectures)
s, *p*, *d*, *f* block elements, the long form of periodic table. Detailed discussion of properties of the elements with reference to *s* and *p*-block. Shielding effect, Slater rules, variation of properties in periodic table. Atomic & Ionic radii (van der Waals), Ionization enthalpy, electron gain enthalpy, Electronegativity, hybridization, group electronegativity. Sanderson's electron density ratio.

Module III: Basics of Organic Chemistry (9 Lectures)
Organic Compounds: Classification, Nomenclature, Hybridization, Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation, Dipole moment. Organic acids and bases. Homolytic and Heterolytic fission, arrow rules, Electrophiles and Nucleophiles; Carbocations, Carbanions, Free radicals and Carbenes. Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Module IV: Chemical Bonding (9 Lectures)
Ionic bond: Radius ratio rule, Packing of ions in crystals. Born-Landé equation, Madelung constant, Born-Haber cycle. *Metallic Bond:* valence bond and band theories, defects in solids. *Weak Chemical Forces:* Van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Hydrogen bonding. *Covalent bond:* Lewis structure, Valence Bond theory, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules, Valence shell electron pair repulsion theory (VSEPR), multiple bonding. Fajan's rules and consequences of polarization.

Module V: Stereochemistry (9 Lectures)
Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: *cis–trans* and, syn-anti isomerism E/Z notations with C.I.P rules.
Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

Text books:
1. Lee, J. D. Concise Inorganic Chemistry ELBS, 1991.
2. Douglas, B. E. and McDaniel, D. H. Concepts & Models of Inorganic Chemistry Oxford, 1970
3. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Reference books:
1. Atkins, P. W. & Paula, J. Physical Chemistry, 10th Ed., Oxford University Press, 2014.
2. Day, M. C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications, 1962.
3. Rodger, G. E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
4. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.

Course code: CH112R1
Course title: General Chemistry- I Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2.0 L: 0 T: 0 P: 3
Class schedule per week: 04
Class: B. Sc.
Level: II
Branch: Chemistry
Name of Teacher:

Syllabus

(A) Titrimetric Analysis

(i) Calibration and use of apparatus

(ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

(i) Estimation of carbonate and hydroxide present together in mixture.

(ii) Estimation of carbonate and bicarbonate present together in a mixture.

(iii) Estimation of free alkali present in different soaps/detergents

(C) Purification of organic compounds by crystallization using the following solvents:

a. Water

b. Alcohol

c. Alcohol-Water

(D) Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)

Reference book:

1. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.
2. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).

Course code: CH213
Course title: General Chemistry-II
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 4 L: 3 T: 1 P: 0
Class schedule per week: 04
Class: B. Sc.
Level: II
Branch: Chemistry
Name of Teacher:

Module-I: States of Matter (9 Lectures)
Gaseous state: Kinetic theory of gas, Maxwell distribution equation, *Ideal & real gases,* compressibility factor, *Z.* Van der Waals equation of state, Boyle temperature. Continuity of states, critical state, law of corresponding states. Liquid state: Physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity. Solid state: Miller indices, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law. Analysis of powder diffraction patterns

Module-II: Ionic Equilibria (9 Lectures)
Strong, moderate and weak electrolytes, degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salt. Qualitative treatment of acid – base titration curves. Theory of acid–bases; Arrhenius, Bronsted Lowry, Lewis concept, SHAB, solvent systems; selection of indicators and their limitations. Hydrolysis and hydrolysis constants.

Module-III: Chemistry of Aromatic Hydrocarbons (9 Lectures)
Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: Isotopic effect, halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism & energy diagram,. Directing effects of the groups.

Module-IV: Oxidation-Reduction (8 Lectures)
Galvanic cells and electrolytic cells, Daniel cell, different kind of half-cells, electromotive forces of a cell and its measurement, Nernst equation, Redox equilibrium, Standard Electrode Potential and its application to inorganic reactions, different types of galvanic cells, Thermodynamics of electrochemical cells and applications, Potentiometric titrations to determine various equilibrium constants.

Module-V: Chemistry of Aliphatic Hydrocarbons (10 Lectures)
Carbon-Carbon sigma bonds: Chemistry of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation. Carbon-Carbon pi bonds: elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, *e.g.* propene, 1-butene, toluene, ethyl benzene. Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes. Alkanes & Cycloalkanes: Types, Conformational Analysis, relative stability & Energy diagrams.

Text books:
1. Kapoor, K. L. A Textbook of Physical Chemistry, Volume 1, Mcmillan Publishers India Ltd, 2004
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 10th Ed., Oxford University Press (2014).
3. Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
1. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

Reference books:
1. Ball, D. W. Physical Chemistry Thomson Press, India (2007).
2. Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
3. Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).
1. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

Course code: CH214R1
Course title: General Chemistry- II Lab
Pre-requisite(s): Intermediate level chemistry
Co- requisite(s):
Credits: 2.0 L: 0 T: 0 P: 3
Class schedule per week: 04
Class: B. Sc.
Level: II
Branch: Chemistry
Name of Teacher:

Syllabus

1. Surface tension measurements.
a. Determine the surface tension by (i) drop number (ii) drop weight method.
b. Study the variation of surface tension of detergent solutions with concentration.
2. Viscosity measurement using Ostwald's viscometer.
3. Indexing of a given powder diffraction pattern of a cubic crystalline system.
4. pH metry
a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
b. Preparation of buffer solutions of different pH
c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.
d. Determination of dissociation constant of a weak acid.
5. Oxidation-Reduction Titrimetry
6. Chromatography
a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
b. Separation of a mixture of two sugars by ascending paper chromatography
c. Separation of a mixture of *o*-and *p*-nitrophenol or *o*-and *p*-aminophenol by thin layer chromatography (TLC)

Reference Books

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
4. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).

CH115 GREEN METHODS IN CHEMISTRY
(Credits: 03:) [L:3; T:0; P:0]

Module-I: Introduction to Green Chemistry; Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

Module-II: Green Chemistry Metrics and their calculations e.g., Atom economy, Atom efficiency, Reaction Mass Intensity and E factor to assess the greenness of the synthesis. Synthesis of Relevant Pharmaceuticals with Greener Approach; Example of a green synthesis of ibuprofen which creates less waste and fewer by products.

Module-III: Biocatalysis; Enzymes for the production of pharmaceuticals, heme-containing cytochrome P450 oxidases, Bioreduction by Microorganisms, synthetic biomimetic metal complexes, Enzymes in the unusual solvents such as supercritical CO2 and ionic liquids

Module-IV: Ultrasound and Microwave Assisted Synthesis: Solvent free microwave assisted organic synthesis, Organic synthesis under microwaves – benefits, limitations, equipment's. Microwave assisted reactions in water: oxidation of toluene to benzoic acid, Microwave assisted reactions in organic solvent: Diels Alder reaction.

Module-V: Relevant Case Studies: Surfactants for Carbon Dioxide– replacing smog producing and ozone depleting solvents with CO2 for precision cleaning and dry cleaning of garments. CO2 as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market. Right-fit pigment: synthetic azopigments to replace toxic organic and inorganic pigments. Green Technique in purification and separation: high performance chromatography and flash chromatography

Reference Books:
1. V. Kumar, An Introduction to Green Chemistry, Vishal Publishing CO. Jalandhar, 2007
4. Kenneth Doxsee, James Hutchison, Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments, Brooks Cole, ISBN: 0534388515.

CH116 FUEL CHEMISTRY
(Credits: 03:) [L:3; T:0; P:0]

Objectives:
The course aims to provide students with a basic scientific and technical understanding of the production, behaviour and handling of hydrocarbon fuels and lubricants, including emerging alternative & renewable fuels. This will enable them to be industry ready to contribute effectively in the field of petroleum chemistry and technology.

Learning Outcomes:
· The course covers both conventional petroleum-based fuels, and alternative & renewable fuels, including gaseous fuels.
· The students will learn the chemistry that underpins petroleum fuel technology, will understand the refining processes used to produce fuels and lubricants and will know how differences in chemical composition affect properties of fuels and their usage in different applications.
· The course will also cover origin of petroleum, crude oil, composition, different refining processes employed industrially to obtain different fractions of petroleum. Further, course will cover various alternative and renewable fuels like Biofuels (Different generations), Gaseous Fuels (e.g. CNG, LNG, CBG, Hydrogen etc.).
· The course will also cover fuel product specifications, various test methods used to qualify different types of fuels as well characterization methods.
· Review of energy scenario (Global & India), Energy sources (renewable and non-renewable).

Module 1:
Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value. Calorific Value Determination.

Module 2:
Coal: Analysis of coal, Proximate and ultimate Analysis, Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas composition and uses. Fractionation of coal tar, uses of coal tar based chemicals, requisites of a good metallurgical coke, Coal gasification (Hydrogasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Module 3:
Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Module 4:
Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Module 5:
Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Reference Books:

- Stocchi, E. *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK (1990).
- Jain, P.C. & Jain, M. *Engineering Chemistry* Dhanpat Rai & Sons, Delhi.

CH219 INTELLECTUAL PROPERTY RIGHTS
(Credits: 03:) [L:3; T:0; P:0]

Objectives:
The course aims to give insights into the basics of the Intellectual Property (IP) and in its wider purview it encompasses intricacies relating to IP. This course is designed to introduce a learning platform to those who may be involved in the making and creation of various forms of IP, besides the effective management of IPR of other creators. The course may also provide cursory understanding of the overall IP ecosystem in the country.

Learning Outcomes:
At the end of this course, students will be able to:
· Learn theoretical concepts of evolution of Intellectual Property Laws, and to differentiate between the different kinds of IP.
Know the existing legal framework relating to IP in India. Comprehend the value of IP and its importance in their respective domains. This course may motivate the students to make their career in multifaceted field of intellectual property rights.

Introduction (Lectures: 6)
Basic concept of Intellectual Property, Rationale behind Intellectual Property, Justifications for protection of IP, IPR and Economic Development, Major International Instruments relating to the protection of IP. The World Intellectual Property Organization (WIPO), WTO and TRIPS Agreement.

Copyright and Related rights (Lectures: 8)
Introduction to copyright and its relevance, subject matter and conditions of protection, ownership and term of copyright, rights under copyright law, infringement of copyright and remedies, exceptions to infringement/ public rights.

Patents (Lectures: 10)
Introduction, Criteria for obtaining patents, Patentable subject matter, Non patentable inventions, Procedure for registration, Term of patent and Rights of patentee, Patent Cooperation Treaty & International registration, Basic concept of Compulsory license and Government use of patent, Infringement of patents and remedies, Software patents and importance for India, Utility model & patent, Trade secrets and know-how agreement, Traditional Knowledge and efforts of Indian Govt. for its protection.

Design and Trademarks (Lectures: 6)
Designs: Meaning of design protection, Concept of original design, Registration &Term of protection, Copyright in Designs. Meaning of mark and Trademark, Categories of Trademark: Service Mark, Certification Mark, Collective Mark, Well known Mark and Non-conventional Mark, Criteria for registrability of trademark: Distinctiveness & non-deceptiveness, A good Trade Mark & its functions, Procedure for registration and Term of protection, Grounds for refusal of trademark registration, Assignment and licensing of marks (Character merchandising), Infringement and Passing Off, Salient Features of Indian Trade Mar Act,1999.

Enforcement and Protection (Lectures: 5)
Enforcement of Intellectual Property Rights: Counterfeiting and Piracy, Understanding Enforcement of IP; and Enforcing IPRs, Enforcement under TRIPS Agreement, Role of Customs and Police in IPR Protection.

References:
1. Pandey, N.; Dhami, K. (2014),Intellectual Property Rights, PHI Learning Pvt. Ltd.
2. Acharya, N.K.(2001),Text Book of Intellectual Property Rights, Asia Law House.
3. Ganguli, P. (2001),Intellectual Property Rights: unleashing the knowledge economy. Tata McGraw Hill.

Additional Resources:
1. https://www.wipo.int
2. Ahuja, V.K.(2017),Law Relating to Intellectual Property Rights, Lexis Nexis.
3. Wadehra, B.L. (2000),Law Relating to Patents, Trade Marks, Copyright, Designs &Geographical Indications. Universal law Publishing Pvt. Ltd..
4. Journal of Intellectual Property Rights (JIPR); NISCAIR(CSIR).

SYLLABUS CHANGE SUMMARY:

SEM	Course Code (Revised)	Course Code	Course Name	Credit	Note# Percentage Change	Page No
I	CH103R1	CH103	Inorganic Chemistry-I; Atomic Structure & Chemical Bonding-I	4	**SM, SN**	
		CH104	Physical Chemistry-I; States of Matter & Ionic Equilibrium	4	**SSM,JD**	
	CH113		Physical Chemistry-I	4		
	CH106R1	CH106	Physical Chemistry-I Lab	2		
II		CH107	Physical Chemistry-II; Chemical Thermodynamics & its Applications	4	**SSM,JD**	
	CH114		Physical Chemistry-II	4		
	CH109	CH109	Physical Chemistry-II Lab	2		
	CH108R1	CH108	Organic Chemistry-I	4	**AP**	
III	CH201R1	CH201	Inorganic Chemistry-II; s and p-Block Elements	4	**SM, SN**	
		CH202	Physical Chemistry-III; Phase Equilibria &Chemical Kinetics	4	**SSM,JD**	
	CH215		**Physical Chemistry-III**			
	CH205R1	CH205	Physical Chemistry-III Lab	2		
	CH216	CH203	Organic Chemistry-II	4	**AP**	
IV	CH 207R1	CH207	Inorganic Chemistry-III; Coordination Chemistry	4	**SM, SN**	
		CH208	**Physical Chemistry-IV; Electrochemistry**	4	**SSM,JD**	
	CH217		**Physical Chemistry-IV**	4		
	CH211R1	CH211	Physical Chemistry-IV Lab	2		
	CH209R1	CH209	Organic Chemistry-III	4	**AP**	
V		CH301	Physical Chemistry-V; Quantum Chemistry & Spectroscopy	4	**SSM, JD**	
	CH326		Physical Chemistry-V	4		
	CH307R1	CH307	Physical Chemistry-V Lab	2		
	CH327	CH302	Organic Chemistry-IV	4	**AP**	
	CH306R1	CH306	Molecular Modeling & Drug Design	4	**JD,DC,AS**	41
		CH312	Molecular Modeling & Drug Design Lab	2	**JD,DC,AS**	
		CH303	Analytical Methods in Chemistry			
VI	CH 313R1	CH313	Inorganic Chemistry-IV; Organometallic Chemistry	4	**SM, SN**	
	CH328	CH314	Organic Chemistry-V	4	**AP**	
VII		CH401	Basic Inorganic Chemistry	4		
	CH402	CH402	Chemical Kinetics & Surface Chemistry	3	**SSM,JD**	
	CH403R1	CH403	Reactions Mechanism in Organic Chemistry	3	**PK**	
	CH404R1	CH404	Organometallic Chemistry	3	**SM, SN**	
	CH405R1	CH405	Principles of Organic Synthesis	4	**PK**	
VIII		CH408	Advanced Inorganic Chemistry	3		
		CH409	Quantum Chemistry & Group Theory	4	**SSM,JD**	
	CH410R1	CH410	Modern Organic Chemistry	3	**PK**	
	CH411	CH411	Equilibrium, Non-Equilibrium & Statistical Thermodynamics	3	**SSM,JD**	
		CH412	Analytical Chemistry	4		
IX		CH501	Spectroscopic Elucidation of Molecular Structure	4		
	CH502R1	CH502	Solid State & Nuclear Chemistry	4	**SM, SN**	
	CH504R1	CH504	Advanced Organic Synthesis	4	**PK**	
X	**CH507R1**	CH507	Selected Topics in Organic Synthesis	4	**PK**	

Note#

- ***Responsible Faculty Members: Please indicate your name (code), if syllabus is revised and proposed with revised subject code.***
- ***If any syllabus/course is missing in above content, please add appropriately in respective semesters.***
- ***Try to adjust font and formatting for one course in one page only for easy visualization and paging.***