

# Syllabus and Lesson Plan of Chemistry

## **B.Sc Hons. (Sem I)**

### **Organic Chemistry 1**

#### **Bonding and Physical Properties (25L)**

**Instructor: Dr. Soumen Mistri**

Valence Bond Theory: Concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding ( $sp^3$ ,  $sp^2$ ,  $sp$ : C-C, C-N & C-O systems and s-cis and s-trans geometry for suitable cases).

Electronic displacements: inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.

MO theory: qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ ,  $n$  – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of  $\pi$  MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about  $\alpha$  and  $\beta$ ; measurement of delocalization energies in terms of  $\beta$  for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

Physical properties: influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.

#### **General Treatment of Reaction Mechanism I (15L)**

Mechanistic classification: ionic, radical and pericyclic (definition and example); reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.

Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

#### **Stereochemistry-I (20L)**

Bonding geometries of carbon compounds and representation of molecules: Tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations.

Concept of chirality and symmetry: symmetry elements and point groups ( $C_v$ ,  $C_{nh}$ ,  $C_{nv}$ ,  $C_n$ ,  $D_h$ ,  $D_{nh}$ ,  $D_{nd}$ ,  $D_n$ ,  $S_n$ (Cs,Ci); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).

Relative and absolute configuration: D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/Z- isomerisms: Optical activity of chiral compounds: optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates); resolution of acids, bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

#### **Practical**

## Separation

Based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, 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 may be of the following types: Benzoic acid/p-Toluidine; p-Nitrobenzoic acid/p- Aminobenzoic acid; p-Nitrotoluene/p-Anisidine; etc.

## Determination of boiling point

Determination of boiling point of common organic liquid compounds e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160°C]

## Identification of a Pure Organic Compound

Solid compounds: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid

Liquid Compounds:

formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene.

## Physical Chemistry I Kinetic Theory and Gaseous state (24 L) Instructor: Mr. Partha Sarathi Mahato

Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Wall collision and rate of effusion

Maxwell's distribution of speed and energy (without derivation): Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy  $\geq \epsilon$ .

Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

## Chemical Thermodynamics (18 L)

Zeroth and 1st law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy 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; Joule's experiment and its consequence.

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

## Chemical kinetics (18 L)

Rate law, order and molecularity:

Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and nth order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)

Role of T and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory

(classical  
**Practical**

treatment)

1. Determination of heat of neutralization of a strong acid by a strong base
2. Study of kinetics of acid-catalyzed hydrolysis of methyl acetate
3. Study of kinetics of decomposition of H<sub>2</sub>O<sub>2</sub>
4. Determination of heat of solution of oxalic acid from solubility measurement

**B.Sc Program (Sem I)**  
**Organic Chemistry-I**  
**Bonding and Physical Properties (25L)**  
**Instructor: Dr. Soumen Mistri**

Valence Bond Theory: Concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding (sp<sup>3</sup>, sp<sup>2</sup>, sp: C-C, C-N & C-O systems and s-cis and s-trans geometry for suitable cases).

Electronic displacements: inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.

MO theory: qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ , n – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of  $\pi$  MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about  $\alpha$  and  $\beta$ ; measurement of delocalization energies in terms of  $\beta$  for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

Physical properties: influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.

**General Treatment of Reaction Mechanism I (15L)**

Mechanistic classification: ionic, radical and pericyclic (definition and example); reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.

Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

**Stereochemistry-I (20L)**

Bonding geometries of carbon compounds and representation of molecules: Tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations. Concept of chirality and symmetry: symmetry elements and point groups (C<sub>v</sub>, C<sub>nh</sub>, C<sub>nv</sub>, C<sub>n</sub>, D<sub>h</sub>, D<sub>nh</sub>, D<sub>nd</sub>, D<sub>n</sub>, S<sub>n</sub>(C<sub>s</sub>, C<sub>i</sub>); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types). Relative and absolute configuration: D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/Z-isomerisms: Optical activity of chiral compounds: optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates); resolution of acids,

bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

### **Practical**

### **Separation**

Based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, 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 may be of the following types: Benzoic acid/p-Toluidine; p-Nitrobenzoic acid/p- Aminobenzoic acid; p-Nitrotoluene/p-Anisidine; etc.

### **Determination of boiling point**

Determination of boiling point of common organic liquid compounds e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160°C]

### **Identification of a Pure Organic Compound**

Solid compounds: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid

Liquid Compounds:

formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

## **B.Sc Hons. (Sem II)**

### **Title: Inorganic Chemistry I**

**Instructor: Dr. Keshab Mondal**

### **Extra nuclear Structure of atom (20L)**

Bohr's theory, its limitations and atomic spectrum of hydrogen atom; Sommerfeld's Theory. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Pauli's Exclusion Principle, Hund's rules and multiplicity, Exchange energy, Aufbau principle and its limitations, Ground state Term symbols of atoms and ions for atomic number upto 30.

### **Chemical periodicity (15L)**

Modern IUPAC Periodic table, Effective nuclear charge, screening effects and penetration, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii, lanthanide contraction. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred- Rochow's scales) and factors influencing these properties, group electronegativities. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements. Secondary periodicity, Relativistic Effect, Inert pair effect.

### **Acid-Base reactions (15L)**

Acid-Base concept: Arrhenius concept, theory of solvent system (in H<sub>2</sub>O, NH<sub>3</sub>, SO<sub>2</sub> and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling's rules. Lux-Flood concept, Lewis concept, group characteristics of Lewis acids, solvent levelling and differentiating effects. Thermodynamic acidity parameters, Drago-Wayland equation. Superacids, Gas phase acidity and proton affinity; HSAB principle. Acid-base

equilibria in aqueous solution (Proton transfer equilibria in water), pH, buffer. Acid-base neutralisation curves; indicator, choice of indicators.

### **Redox Reactions and precipitation reactions (10L)**

Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Influence of complex formation, precipitation and change of pH on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples) Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides.

### **Practical**

#### **Acid and Base Titrations**

1. Estimation of carbonate and hydroxide present together in mixture
2. Estimation of carbonate and bicarbonate present together in a mixture.
3. Estimation of free alkali present in different soaps/detergents.

#### **Oxidation-Reduction Titrimetric**

1. Estimation of Fe(II) using standardized  $\text{KMnO}_4$  solution
2. Estimation of oxalic acid and sodium oxalate in a given mixture
3. Estimation of Fe(II) and Fe(III) in a given mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$  solution.
4. Estimation of Fe(III) and Mn(II) in a mixture using standardized  $\text{KMnO}_4$  solution
5. Estimation of Fe(III) and Cu(II) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .
6. Estimation of Fe(III) and Cr(III) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .

**Title: Organic Chemistry II**  
**Instructor: Dr. Soumen Mistri**

### **Stereochemistry II (22L)**

1. Chirality arising out of stereocenter: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidenecycloalkanes and biphenyls; related configurational descriptors (R/S and P/M); atropisomerism; racemisation of chiral biphenyls; buttressing effect.
2. Concept of prostereoisomerism: prostereogenic centre; concept of (pro)n-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and R/S descriptors; pro-r and pro-s descriptors of ligands on propseudoasymmetric centre.
3. Conformation: conformational nomenclature: eclipsed, staggered, gauche, syn and anti; dihedral angle, torsion angle; Klyne-Prelog terminology; P/M descriptors; energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; butane gauche interaction; conformational analysis of ethane, propane, n-butane,
4. 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (s-cis and s-trans).

### **General Treatment of Reaction Mechanism II (22L)**

1. Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.
2. Concept of organic acids and bases: effect of structure, substituent and solvent on acidity and basicity; proton sponge; gas-phase acidity and basicity; comparison between nucleophilicity and basicity; HSAB principle; application of thermodynamic principles in acid-base equilibria.
3. Tautomerism: prototropy (keto-enol, nitro - aci-nitro, nitroso-oximino, diazo-amino and enamine-imine systems); valence tautomerism and ring-chain tautomerism; composition of the equilibrium in different systems (simple carbonyl; 1,2- and 1,3-dicarbonyl systems, phenols and related systems), factors affecting keto-enol tautomerism; application of thermodynamic principles in tautomeric equilibria.
4. Reaction kinetics: rate constant and free energy of activation; concept of order and molecularity; free energy profiles for one-step, two-step and three-step reactions; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect: primary and secondary kinetic isotopic effect (kH /kD); principle of microscopic reversibility; Hammond's postulate.

### **Substitution and Elimination Reactions (16L)**

1. Free-radical substitution reaction: halogenation of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.
2. Nucleophilic substitution reactions: substitution at  $sp^3$  centre: mechanisms (with evidence), relative rates & stereochemical features:  $SN_1$ ,  $SN_2$ ,  $SN_2'$ ,  $SN_1'$  (allylic rearrangement) and  $SN_i$ ; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP; role of crown ethers and phase transfer catalysts; [systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides].
3. Elimination reactions:  $E_1$ ,  $E_2$ ,  $E_1cB$  and  $E_i$  (pyrolytic syn eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination; importance of Bredt's rule relating to the formation of  $C=C$ .

### **Practical**

#### **Organic Preparations**

A. The following reactions are to be performed, noting the yield of the crude product:

1. Nitration of aromatic compounds
2. Condensation reactions
3. Hydrolysis of amides/imides/esters
4. Acetylation of phenols/aromatic amines
5. Benzoylation of phenols/aromatic amines
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

Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.

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.

### **B.Sc Program (Sem II)**

#### **Title: Inorganic Chemistry-I**

**Instructor: Dr. Keshab Mondal**

### **Syllabus:**

#### **Theory**

#### **Extra nuclear Structure of atom (20L)**

Bohr's theory, its limitations and atomic spectrum of hydrogen atom; Sommerfeld's Theory. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Pauli's Exclusion Principle, Hund's rules and multiplicity, Exchange energy, Aufbau principle and its limitations, Ground state Term symbols of atoms and ions for atomic number upto 30.

#### **Chemical periodicity (15L)**

Modern IUPAC Periodic table, Effective nuclear charge, screening effects and penetration, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii, lanthanide contraction. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred-Rochow's scales) and factors influencing these properties, group electronegativities. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements. Secondary periodicity, Relativistic Effect, Inert pair effect.

### **Acid-Base reactions (15L)**

Acid-Base concept: Arrhenius concept, theory of solvent system (in H<sub>2</sub>O, NH<sub>3</sub>, SO<sub>2</sub> and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling's rules. Lux-Flood concept, Lewis concept, group characteristics of Lewis acids, solvent levelling and differentiating effects. Thermodynamic acidity parameters, Drago-Wayland equation. Superacids, Gas phase acidity and proton affinity; HSAB principle. Acid-base equilibria in aqueous solution (Proton transfer equilibria in water), pH, buffer. Acid-base neutralisation curves; indicator, choice of indicators.

### **Redox Reactions and precipitation reactions (10L)**

Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Influence of complex formation, precipitation and change of pH on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples) Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides.

### **Practical**

#### **Acid and Base Titrations**

1. Estimation of carbonate and hydroxide present together in mixture
2. Estimation of carbonate and bicarbonate present together in a mixture.
3. Estimation of free alkali present in different soaps/detergents.

#### **Oxidation-Reduction Titrimetric**

1. Estimation of Fe(II) using standardized KMnO<sub>4</sub> solution
2. Estimation of oxalic acid and sodium oxalate in a given mixture
3. Estimation of Fe(II) and Fe(III) in a given mixture using K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solution.
4. Estimation of Fe(III) and Mn(II) in a mixture using standardized KMnO<sub>4</sub> solution
5. Estimation of Fe(III) and Cu(II) in a mixture using K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.
6. Estimation of Fe(III) and Cr(III) in a mixture using K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.

### **B.Sc Hons. (SemIII)**

#### **Title:Physical Chemistry II**

**Instructor: Mr. Partha Sarathi Mahato**

### **Syllabus:**

#### **Theory**

#### **Transport processes (16 L)**

1. Diffusion; Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties.
2. Viscosity: General features of fluid flow (streamline flow and turbulent flow); Newton's equation, viscosity coefficient; Poiseuille's equation; principle of determination of viscosity coefficient of liquids by falling sphere method; Temperature variation of viscosity of liquids and comparison with that of gases.

3. Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye –Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations.
4. Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule.

#### **Applications of Thermodynamics – I (24L)**

1. Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of  $\Delta Q/T$  and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; Auxiliary state functions (G and A) and their variation with T, P and V. Criteria for spontaneity and equilibrium.
2. Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations
3. Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential ( $\mu$ ) with temperature and pressure; Gibbs-Duhem equation; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S, H and V during mixing for binary solutions
4. Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of  $K_P$ ,  $K_C$  and  $K_X$ ; van't Hoff's reaction isobar and isochore from different standard states; Shifting of equilibrium due to change in external parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle and its derivation
5. Dissociation of weak electrolyte. Solubility equilibrium
6. Nernst's distribution law; Application- (finding out  $K_{eq}$  using Nernst dist law for  $KI + I_2 = KI_3$  and dimerization of benzene)

#### **Foundation of Quantum Mechanics (20L)**

1. Beginning of Quantum Mechanics: Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (without proof)
2. Wave function: Schrodinger time-independent equation; nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function
3. Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear operators; Commutation of operators, commutator and uncertainty relation; Expectation value; Hermitian operator; Postulates of Quantum Mechanics
4. Particle in a box: Setting up of Schrodinger equation for one-dimensional box and its solution; Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution); Expectation values of  $x$ ,  $x^2$ ,  $p_x$  and  $p_x^2$  and their significance in relation to the uncertainty principle; Extension of the problem to two and three dimensions and the concept of degenerate energy levels
5. Simple Harmonic Oscillator: setting up of the Schrodinger stationary equation, energy expression (without derivation), expression of wave function for  $n = 0$  and  $n = 1$  (without derivation) and their characteristic features

#### **Practical**

1. Study of viscosity of unknown liquid (glycerol, sugar) with respect to water
2. Determination of partition coefficient for the distribution of  $I_2$  between water and  $CHCl_3$
3. Determination of  $K_{eq}$  for  $KI + I_2 = KI_3$ , using partition coefficient between water and  $CHCl_3$
4. Conductometric titration of an acid (strong, weak/ monobasic, dibasic) against base strong



5. Study of saponification reaction conductometrically
6. Verification of Ostwald's dilution law and determination of  $K_a$  of weak acid

**Title: Inorganic Chemistry II**  
**Instructor: Dr. Keshab Mondal**

**Chemical Bonding-I (20L)**

1. Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its application and 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. Defects in solids (elementary idea). Solubility energetics of dissolution process.
2. Covalent bond: Polarizing power and polarizability, ionic potential, Fajan's rules. Lewis structures, formal charge. Valence Bond Theory. The hydrogen molecule (Heitler-London approach), directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, Dipole moments, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry) and multiple bonding ( $\sigma$  and  $\pi$  bond approach).

**Chemical Bonding-II (25L)**

1. Molecular orbital concept of bonding (The approximations of the theory, Linear combination of atomic orbitals (LCAO)) (elementary pictorial approach): sigma and pi- bonds and delta interaction, multiple bonding. Orbital designations: gerade, ungerade, HOMO, LUMO. Orbital mixing. MO diagrams of  $H_2$ ,  $Li_2$ ,  $Be_2$ ,  $B_2$ ,  $C_2$ ,  $N_2$ ,  $O_2$ ,  $F_2$ , and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO,  $NO^+$ ,  $CN^-$ , HF,  $BeH_2$ ,  $CO_2$  and  $H_2O$ . Bond properties: bond orders, bond lengths.
2. Metallic Bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.
3. Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Intermolecular forces: Hydrogen bonding (theories of hydrogen bonding, valence bond treatment), receptor-guest interactions, Halogen bonds. Effects of chemical force, melting and boiling points.

**Radioactivity (15L)**

1. Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers.
2. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes.
3. Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

**Practical**

**Iodo / Iodimetric Titrations**

1. Estimation of Cu(II)
2. Estimation of Vitamin C
3. Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
4. Estimation of available chlorine in bleaching powder

**Estimation of metal content in some selective samples**

1. Estimation of Cu in brass.
2. Estimation of Cr and Mn in Steel.
3. Estimation of Fe in cement.

**Title: Organic Chemistry III**

**Instructor: Dr. Soumen Mistri**

**Chemistry of alkenes and alkynes (12L)**

1. Addition to  $C=C$ : mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity; reactions: hydrogenation, halogenations, iodolactonisation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, syn and anti-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; 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; interconversion of E - and Z - alkenes; contra-thermodynamic isomerization of internal alkenes.

2. Addition to  $C\equiv C$  (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.

#### **Aromatic Substitution (10L)**

1. Electrophilic aromatic substitution: mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmidt); Ipso substitution.

2. Nucleophilic aromatic substitution: addition-elimination mechanism and evidences in favour of it;  $SN1$  mechanism; cine substitution (benzyne mechanism), structure of benzyne.

#### **Carbonyl and Related Compounds (30L)**

1. Addition to  $C=O$ : structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; Burgi-Dunitz trajectory in nucleophilic additions; formation of hydrates, cyano hydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen-based nucleophiles; 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.

2. Exploitation of acidity of  $\alpha$ -H of  $C=O$ : formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation,  $SeO_2$  (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, aza-enolates and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

3. Elementary ideas of Green Chemistry: Twelve (12) principles of green chemistry; planning of green synthesis; common organic reactions and their counterparts: reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.

4. Nucleophilic addition to  $\alpha,\beta$ -unsaturated carbonyl system: general principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Stetter reaction, Robinson annulation.

5. Substitution at  $sp^2$  carbon ( $C=O$  system): mechanism (with evidence):  $BAC2$ ,  $AAC2$ ,  $AAC1$ ,  $AAL1$  (in connection to acid and ester); acid derivatives: amides, anhydrides & acyl halides (formation and hydrolysis including comparison).

#### **Organometallics (8L)**

Grignard reagent; Organolithiums; 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, 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 and base-nucleophile dichotomy in case of organometallic reagents.

#### **Practical**

##### **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:

4. aromatic amino ( $-\text{NH}_2$ ), aromatic nitro ( $-\text{NO}_2$ ), amido ( $-\text{CONH}_2$ , including imide), phenolic – OH, carboxylic acid ( $-\text{COOH}$ ), carbonyl ( $-\text{CHO}$  and  $>\text{C}=\text{O}$ ); only one test for each functional group is to be reported.

5. Melting point of the given compound

6. Preparation, purification and melting point determination of a crystalline derivative of the given compound

7. Identification of the compound through literature survey.

Each student, during laboratory session, is required to carry out qualitative chemical tests for all the special elements and the functional groups with relevant derivatisation in known and unknown (at least six) organic compounds

### **Title: Basic Analytical Chemistry**

**Instructor: Dr. Soumen Mistri**

#### **Theory (30L)**

##### **Introduction**

Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation of experimental data and results, from the point of view of significant figures.

##### **Analysis of soil**

Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

1. Determination of pH of soil samples.

2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

##### **Analysis of water**

Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

1. Determination of pH, acidity and alkalinity of a water sample.

2. Determination of dissolved oxygen (DO) of a water sample.

##### **Analysis of food products**

Nutritional value of foods, idea about food processing and food preservations and adulteration.

1. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.

2. Analysis of preservatives and colouring matter.

##### **Chromatography**

Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

1. Paper chromatographic separation of mixture of metal ion ( $\text{Fe}^{3+}$  and  $\text{Al}^{3+}$ ).

2. To compare paint samples by TLC method.

##### **Ion-exchange**

1. Column, ion-exchange chromatography etc.

2. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

##### **Analysis of cosmetics**

Major and minor constituents and their function

1. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.

2. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration

##### **Suggested Applications (Any one)**

1. To study the use of phenolphthalein in trap cases.

2. To analyse arson accelerants.

3. To carry out analysis of gasoline.

##### **Suggested Instrumental demonstrations**

1. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.

2. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.

3. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drinks

**B.Sc Program (Sem III)**

**Title: Physical Chemistry-I**

**Instructor: Mr. Partha Sarathi Mahato**

**Kinetic Theory and Gaseous state (24 L)**

1. Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Wall collision and rate of effusion
2. Maxwell's distribution of speed and energy (without derivation): Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy  $\geq \epsilon$ .
3. Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

**Chemical Thermodynamics (18 L)**

1. Zeroth and 1st law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy 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; Joule's experiment and its consequence
2. Thermochemistry: Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

**Chemical kinetics (18 L)**

1. Rate law, order and molecularity:  
Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and nth order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)
2. Role of T and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

**Practical**

1. Determination of heat of neutralization of a strong acid by a strong base
2. Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

3. Study of kinetics of decomposition of  $\text{H}_2\text{O}_2$
4. Determination of heat of solution of oxalic acid from solubility measurement

**B.Sc Hons. (Sem IV)**

**Title: Physical Chemistry III**

**Instructor: Mr. Partha Sarathi Mahato**

**Applications of Thermodynamics – II (20L)**

1. Binary mixture: Chemical potential of individual components. Thermodynamic parameters of mixing ideal solution; Colligative properties: Vapour pressure of solution; Ideal solutions, ideally diluted solutions and colligative properties; Raoult's law; Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) Osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution; Abnormal colligative properties
2. Phase rule: Definitions of phase, component and degrees of freedom; Phase rule and its derivations; Definition of phase diagram; Phase diagram for water,  $\text{CO}_2$ , Sulphur
3. First order phase transition and Clapeyron equation; Clausius-Clapeyron equation - derivation and use; Liquid vapour equilibrium for two component systems; Phenol-water system
4. Binary solutions: Ideal solution; Positive and negative deviations from ideal behaviour; Principle of fractional distillation; Duhem-Margules equation; Henry's law; Konowaloff's rule; Azeotropic solution; Liquid-liquid phase diagram using phenol- water system; Solid-liquid phase diagram; Eutectic mixture

**Applications of Thermodynamics – III (20L)**

1. Ionic equilibria: Chemical potential of an ion in solution; Activity and activity coefficients of ions in solution; Debye-Huckel limiting law-brief qualitative description of the postulates involved, qualitative idea of the model, the equation (without derivation) for ion-ion atmosphere interaction potential. Estimation of activity coefficient for electrolytes using Debye-Huckel limiting law; Mean ionic activity coefficient; Applications of the Debye-Huckel equation and its limitations.
2. Electromotive Force: Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry; 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. 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  $\text{SbO/Sb}_2\text{O}_3$  electrodes
3. 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)

**Surface & nanoscience (20L)**

1. Surface tension and energy: Surface tension, surface energy, excess pressure, capillary rise and surface tension; Work of cohesion and adhesion, spreading of liquid over other surface; Vapour pressure over curved surface; Temperature dependence of surface tension
2. Adsorption: Physical and chemical adsorption; Freundlich and Langmuir adsorption isotherms; multilayer adsorption and BET isotherm (no derivation required); Gibbs adsorption isotherm and surface excess; Heterogeneous catalysis (single reactant); Zero order and fractional order reactions;
3. Colloids: Lyophobic and lyophilic sols, Origin of charge and stability of lyophobic colloids, Coagulation and Schulz-Hardy rule, Zeta potential and Stern double layer (qualitative idea), Tyndall effect; Electrokinetic phenomena (qualitative idea only); Determination of Avogadro number by Perrin's method; Stability of colloids and zeta potential; Micelle formation

4. Nanomaterials: Importance of nano-systems; confinement and dimensionality with example (dot, wire etc.); Different approaches for preparation of nanomaterials.

#### **Practical**

1. Determination of solubility of sparingly soluble salt in water, in electrolyte with common ions and in neutral electrolyte (using common indicator)
2. Potentiometric titration: (a) weak acid vs. base, (b) Redox, determination of  $E^0$
3. Study of phenol-water phase diagram
4. Spectrophotometric determination of CMC
5. Determination of surface tension of a liquid using Stalagmometer

### **Title: Inorganic Chemistry III**

**Instructor: Dr. Keshab Mondal**

#### **General Principles of Metallurgy (10L)**

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

#### **Chemistry of s and p Block Elements (18L)**

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Beryllium hydrides and halides. Boric acid and borates, boron nitrides, borohydrides (diborane) and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, phosphorus, sulphur and chlorine. Peroxo acids of sulphur, sulphur-nitrogen compounds, interhalogen compounds, polyhalide ions, pseudohalogens, fluorocarbons and basic properties of halogens.

#### **Noble Gases (10L)**

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of  $\text{XeF}_2$ ,  $\text{XeF}_4$  and  $\text{XeF}_6$ ; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for  $\text{XeF}_2$  and  $\text{XeF}_4$ ). Xenon-oxygen compounds. Molecular shapes of noble gas compounds (VSEPR theory).

#### **Inorganic Polymers (10L)**

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes.

#### **Coordination Chemistry-I (12L)**

Coordinate bonding: double and complex salts. Werner's theory of coordination complexes, Classification of ligands, Ambidentate ligands, chelates, Coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), Isomerism in coordination compounds, constitutional and stereo isomerism, Geometrical and optical isomerism in square planar and octahedral complexes.

#### **Practical**

##### **Complexometric titration**

1.  $\text{Zn(II)}$
2.  $\text{Zn(II)}$  in a  $\text{Zn(II)}$  and  $\text{Cu(II)}$  mixture.
3.  $\text{Ca(II)}$  and  $\text{Mg(II)}$  in a mixture.

4. Hardness of water.

**Inorganic preparations**

1.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
2. Cis and trans  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
3.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
4. Cis and trans  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
5. Potassium dioxalatodiaquachromate(III)
6. Tetraamminecarbonatocobalt (III) ion
7. Potassium tris(oxalate)ferrate(III)
8. Tris-(ethylenediamine) nickel(II) chloride.
9.  $[\text{Mn}(\text{acac})_3]$  and  $[\text{Fe}(\text{acac})_3]$  (acac= acetylacetonate)

**Title: Organic Chemistry IV**

**Instructor: Mr. Partha Sarathi Mahato**

**Nitrogen compounds (12L)**

1. Amines: Aliphatic & Aromatic: preparation, separation (Hinsberg's method) and identification of primary, secondary and tertiary amines; reaction (with mechanism): Eschweiler-Clarke methylation, diazo coupling reaction, Mannich reaction; formation and reactions of phenylenediamines, diazomethane and diazoacetic ester.
2. Nitro compounds (aliphatic and aromatic): preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis, Henry reaction and conjugate addition of nitroalkane anion.
3. Alkyl nitrile and isonitrile: preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.
4. Diazonium salts and their related compounds: reactions (with mechanism) involving replacement of diazo group; reactions: Gomberg, Meerwein, Japp-Klingermann.

**Rearrangements (16L)**

Mechanism with evidence and stereochemical features for the following:

1. Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzil- benzilic acid rearrangement, Demjanov rearrangement, Tiffeneau-Demjanov rearrangement.
2. Rearrangement to electron-deficient nitrogen: rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann.
3. Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, cumene hydroperoxide-phenol rearrangement and Dakin reaction.
4. Aromatic rearrangements: Migration from oxygen to ring carbon: Fries rearrangement and Claisen rearrangement.
5. Migration from nitrogen to ring carbon: Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.
6. Rearrangement reactions by green approach: Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

**The Logic of Organic Synthesis (12L)**

1. Retrosynthetic analysis: disconnections; synthons, donor and acceptor synthons; natural reactivity and umpolung; latent polarity in bifunctional compounds: consonant and dissonant polarity; illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and addition (FGI and FGA); C-C disconnections and synthesis: one-group and two-group (1,2- to 1,5-dioxygenated compounds), reconnection (1,6-dicarbonyl); protection-deprotection strategy (alcohol, amine, carbonyl, acid).
2. Strategy of ring synthesis: thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.
3. Asymmetric synthesis: stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity (only definition); enantioselectivity: kinetically controlled MPV reduction;



diastereoselectivity: addition of nucleophiles to C=O adjacent to a stereogenic centre: Felkin-Anh and Zimmermann-Traxler models.

### **Organic Spectroscopy (20L)**

1. UV Spectroscopy: introduction; types of electronic transitions, end absorption; transition dipole moment and allowed/forbidden transitions; chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper-/Hypochromic effects); application of Woodward's Rules for calculation of  $\lambda_{\text{max}}$  for the following systems: conjugated diene,  $\alpha,\beta$ -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of  $\lambda_{\text{max}}$  considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.
2. IR Spectroscopy: introduction; modes of molecular vibrations (fundamental and non-fundamental); IR active molecules; application of Hooke's law, force constant; fingerprint region and its significance; effect of deuteration; overtone bands; vibrational coupling in IR; 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 $\equiv$ C, C $\equiv$ N; characteristic/diagnostic bending vibrations are included; factors affecting stretching frequencies: effect of conjugation, electronic effects, mass effect, bond multiplicity, ring-size, solvent effect, H-bonding on IR absorptions; application in functional group analysis.
3. NMR Spectroscopy: introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance 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; elementary idea about non-first-order splitting; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic); rapid proton exchange; interpretation of NMR spectra of simple compounds.
4. Applications of IR, UV and NMR spectroscopy for identification of simple organic molecules.

### **Practical**

1. Estimation of glycine by Sørensen'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 vitamin-C (reduced)
5. Estimation of aromatic amine (aniline) by bromination (Bromate-Bromide) method
6. Estimation of phenol by bromination (Bromate-Bromide) method
7. Estimation of formaldehyde (Formalin)
8. Estimation of acetic acid in commercial vinegar
9. Estimation of urea (hypobromite method)
10. Estimation of saponification value of oil/fat/ester

**Title: Analytical Clinical Biochemistry**

**Instructor: Mr. Partha Sarathi Mahato**

### **Theory (30L)**

#### **Review of Concepts from Core Course**

1. Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle. Isolation and characterization of polysaccharides.
2. Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins:  $\alpha$ -helix and  $\beta$ -pleated sheets, Isolation, characterization, denaturation of proteins.



3. Enzymes: Nomenclature, Characteristics (mention of Ribozymes), and Classification; Active site, Mechanism of enzyme action, Stereospecificity of enzymes, Coenzymes and cofactors, Enzyme inhibitors, Introduction to Biocatalysis: Importance in "Green Chemistry" and Chemical Industry.

4. Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications. Lipoproteins. Properties, functions and biochemical functions of steroid hormones. Biochemistry of peptide hormones.

5. Structure of DNA (Watson-Crick model) and RNA, Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation, Introduction to Gene therapy.

6. Enzymes: Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.

**Biochemistry of disease: A diagnostic approach by blood/ urine analysis.**

1. Blood: Composition and functions of blood, blood coagulation. Blood collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

2. Urine: Collection and preservation of samples. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

**Hands On Practical**

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.
2. Lipids – qualitative.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Determination of cholesterol using Liebermann- Burchard reaction.
6. Proteins – qualitative.
7. Isolation of protein.
8. Determination of protein by the Biuret reaction.
9. Determination of nucleic acids

**B.Sc Program (Sem IV)**

**Title: Inorganic Chemistry-III**

**Instructor: Dr. Keshab Mondal**

**General Principles of Metallurgy (10L)**

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining.

**Chemistry of s and p Block Elements (18L)**

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Beryllium hydrides and halides. Boric acid and borates, boron nitrides, borohydrides (diborane) and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, phosphorus, sulphur and chlorine. Peroxo acids of sulphur, sulphur-nitrogen compounds, interhalogen compounds, polyhalide ions, pseudohalogens, fluorocarbons and basic properties of halogens.

**Noble Gases (10L)**

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub>; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF<sub>2</sub> and XeF<sub>4</sub>). Xenon-oxygen compounds. Molecular shapes of noble gas compounds (VSEPR theory).

**Inorganic Polymers (10L)**

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes.

### **Coordination Chemistry-I (12L)**

Coordinate bonding: double and complex salts. Werner's theory of coordination complexes, Classification of ligands, Ambidentate ligands, chelates, Coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), Isomerism in coordination compounds, constitutional and stereo isomerism, Geometrical and optical isomerism in square planar and octahedral complexes.

#### **Practical**

##### **Complexometric titration**

1. Zn(II)
2. Zn(II) in a Zn(II) and Cu(II) mixture.
3. Ca(II) and Mg(II) in a mixture.
4. Hardness of water.

##### **Inorganic preparations**

1.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
2. Cis and trans  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
3.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
4. Cis and trans  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
5. Potassium dioxalatodiaquachromate(III)
6. Tetraamminecarbonatocobalt (III) ion
7. Potassium tris(oxalate)ferrate(III)
8. Tris-(ethylenediamine) nickel(II) chloride.
9.  $[\text{Mn}(\text{acac})_3]$  and  $[\text{Fe}(\text{acac})_3]$  (acac= acetylacetonate)

### **B.Sc Hons. (Sem V)**

#### **Title: Inorganic Chemistry IV**

**Instructor: Dr. Keshab Mondal**

### **Coordination Chemistry-II (30L)**

VB description and its limitations. Elementary Crystal Field Theory: splitting of dn configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy (CFSE) in weak and strong fields; pairing energy. Spectrochemical series. Jahn- Teller distortion. Octahedral site stabilization energy (OSSE). Metal-ligand bonding (MO concept, elementary idea), sigma- and pi- bonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals (examples). Magnetism and Colour: Orbital and spin magnetic moments, spin only moments of dn ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for 3d1 to 3d9 ions. Racah parameter. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

### **Chemistry of d- and f- block elements (30L)**

#### **Transition Elements:**

General comparison of 3d, 4d and 5d elements in term of electronic configuration, oxidation states, redox properties, coordination chemistry.

#### **Lanthanoids and Actinoids:**

General Comparison on Electronic configuration, oxidation states, colour, spectral and magnetic properties; lanthanide contraction, separation of lanthanides (ion-exchange method only).

#### **Practical**

##### **Chromatography of metal ions**

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

1. Ni (II) and Co (II)

## 2. Fe (III) and Al (III)

### Gravimetry

1. Estimation of nickel (II) using Dimethylglyoxime (DMG).
2. Estimation of copper as CuSCN
3. Estimation of Al (III) by precipitating with oxine and weighing as Al(oxine)<sub>3</sub> (aluminium oxinate)
4. Estimation of chloride

### Spectrophotometry

1. Measurement of 10Dq by spectrophotometric method.
2. Determination of max of [Mn(acac)<sub>3</sub>] and [Fe(acac)<sub>3</sub>] complexes

**Title: Organic Chemistry V**

**Instructor: Dr. Soumen Mistri**

### Carbocycles and Heterocycles

1. Polynuclear hydrocarbons and their derivatives: 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, phenanthrene and their derivatives.
2. 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: Hantzsch synthesis; 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 approach and mechanistic details): indole: Fischer, Madelung and Reissert; quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: Bischler-Napieralski synthesis.

### Cyclic Stereochemistry

Alicyclic compounds: concept of I-strain; conformational analysis: cyclohexane, mono and disubstituted cyclohexane; symmetry properties and optical activity; topomerisation; ring-size and ease of cyclisation; conformation & reactivity in cyclohexane system: consideration of steric and stereoelectronic requirements; elimination (E2, E1), nucleophilic substitution (SN1, SN2, SNi, NGP), merged substitution-elimination; rearrangements; oxidation of cyclohexanol, esterification, saponification, lactonisation, epoxidation, pyrolytic syn elimination and fragmentation reactions.

### Pericyclic reactions

Mechanism, stereochemistry, regioselectivity in case of

1. Electrocyclic reactions: FMO approach involving 4 $\pi$ - and 6 $\pi$ -electrons (thermal and photochemical) and corresponding cycloreversion reactions.
2. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.
3. 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.

### Carbohydrates

1. 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<sub>3</sub> oxidation, selective oxidation of terminal -CH<sub>2</sub>OH of aldoses, reduction to alditols, 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.

### 2. Disaccharides:

Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar.

3. Polysaccharides: starch (structure and its use as an indicator in titrimetric analysis).

### Biomolecules

1. Amino acids: synthesis with mechanistic details: Strecker, Gabriel, acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine; isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.
2. Peptides: 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 unit determination (Edman, Sanger & 'dansyl' methods); partial hydrolysis; specific cleavage of peptides: use of CNBr.
3. Nucleic acids: pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalysed hydrolysis of nucleosides (both pyrimidine and purine types); comparison of alkaline hydrolysis of DNA and RNA; elementary idea of double helical structure of DNA (Watson-Crick model); complimentary base-pairing in DNA.

### ***Practical***

#### **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 leaf pigments from spinach leaves
4. Column chromatographic separation of mixture of dyes
5. Paper chromatographic separation of a mixture containing 2/3 amino acids
6. Paper chromatographic separation of a mixture containing 2/3 sugars

#### **Spectroscopic Analysis of Organic Compounds**

1. Assignment of labelled peaks in the  $^1\text{H}$  NMR spectra of the known organic compounds explaining the relative  $\delta$ -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 $\equiv$ C, C $\equiv$ 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:
  - a. 4-Bromoacetanilide
  - b. 2-Bromo-4'-methylacetophenone
  - c. Vanillin
  - d. 2-Methoxyacetophenone
  - e. 4-Aminobenzoic acid
  - f. Salicylamide
  - g. 2-Hydroxyacetophenone
  - h. 1,3-Dinitrobenzene
  - i. Benzylacetate
  - j. trans-4-Nitrocinnamaldehyde
  - k. Diethyl fumarate
  - l. 4-Nitrobenzaldehyde
  - m. 4-Methylacetanilide
  - n. Mesityl oxide
  - o. 2-Hydroxybenzaldehyde
  - p. 4-Nitroaniline
  - q. 2-Hydroxy-3-nitrobenzaldehyde
  - r. 2,3-Dimethylbenzonitrile
  - s. Pent-1-yn-3-ol
  - t. 3-Nitrobenzaldehyde
  - u. 3-Ethoxy-4-hydroxybenzaldehyde
  - v. 2-Methoxybenzaldehyde
  - w. Methyl 4-hydroxybenzoate
  - x. Methyl 3-hydroxybenzoate
  - y. 3-Aminobenzoic acid
  - z. Ethyl 3-aminobenzoate
  - aa. Ethyl 4-aminobenzoate
  - bb. 3-nitroanisole
  - cc. 5-Methyl-2-nitroanisole
  - dd. 3-Methylacetanilide

**Title: Advanced Physical Chemistry**

**Instructor: Mr. Partha Sarathi Mahato**

**Crystal Structure (15L)**

1. Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography (Haüy's law and Steno's law); Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice.
2. Crystal planes: Distance between consecutive planes [cubic, tetragonal and orthorhombic lattices]; Indexing of planes, Miller indices; calculation of  $d_{hkl}$ ; Relation between molar mass and unit cell dimension for cubic system;
3. Diffraction of X-ray by crystals, Laue equation, reciprocal lattice, Bragg equation, determination of crystal structure: Powder method; Structure of NaCl and KCl crystals, elementary idea of structure factor.

### **Statistical Thermodynamics (12L)**

1. Configuration: Macrostates, microstates and configuration; calculation with harmonic oscillator; variation of  $W$  with  $E$ ; equilibrium configuration
2. Boltzmann distribution: Thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation); Applications to barometric distribution
3. Partition function: molecular partition function and thermodynamic properties, Maxwell's speed distribution; Gibbs' paradox

### **Third law of thermodynamics and properties near 0K (15L)**

1. Specific heat of solid: Coefficient of thermal expansion, thermal compressibility of solids; Dulong –Petit's law; Equipartition theorem and heat capacities; Perfect Crystal model, Einstein's theory – derivation from partition function, limitations; Debye's  $T^3$  law – analysis at the two extremes
2. 3rd law: Absolute entropy, Planck's law, Calculation of entropy, Nernst heat theorem
3. Adiabatic demagnetization: Approach to zero Kelvin.

### **Quantum Chemistry (18L)**

1. 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
2. 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; Orbitals and their shapes; Setting up of Schrödinger equation for many-electron atoms (He, Li), atomic units

#### ***Practical***

Computer Programming 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

**Title: Inorganic Materials of Industrial Importance**  
**Silicate Industries (15L)**

**Instructor: Dr. Keshab Mondal**

1. 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.

2. 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.

3. Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

#### **Fertilizers (6L)**

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.

#### **Surface Coatings (15L)**

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.

#### **Batteries (8L)**

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.

#### **Alloys (6L)**

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 (Ar and heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

#### **Catalysis (6L)**

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.

#### **Chemical explosives(4L)**

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

#### **Practical**

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).

#### **B.Sc Program (Sem V)**

### **Title: Inorganic Materials of Industrial Importance**

**Instructor: Dr. Keshab Mondal**

#### **Silicate Industries (15L)**

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.

#### **Fertilizers (6L)**

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.

#### **Surface Coatings (15L)**

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.

#### **Batteries (8L)**

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.

#### **Alloys (6L)**

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 (Ar and heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

#### **Catalysis (6L)**

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.

#### **Chemical explosives(4L)**

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

#### **Practical**

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).

#### **B.Sc Hons. (Sem VI)**

#### **Title:Inorganic Chemistry V**

**Instructor: Dr. Keshab Mondal**

#### **Bioinorganic Chemistry (20L)**

Elements of life: essential and beneficial elements, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, Fe<sup>3+/2+</sup>, Cu<sup>2+/+</sup>, and Zn<sup>2+</sup>). Metal ion transport across biological membrane Na<sup>+</sup>/ K<sup>+</sup>-ion pump. Dioxygen molecule in life. Dioxygen management proteins: Haemoglobin, Myoglobin, Hemocyanine and Hemerythrin. Electron transfer proteins: Cytochromes and Ferredoxins. Hydrolytic enzymes: carbonate bicarbonate buffering system and carbonic anhydrase and carboxyanhydrase A. Biological nitrogen fixation, Photosynthesis: Photosystem-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases (examples only)

#### **Organometallic Chemistry (18L)**

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. 18-electron and 16-electron rules (pictorial MO approach). Applications of 18-electron rule to metal carbonyls, nitrosyls, cyanides. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls. pi-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding.

Zeise's salt: Preparation, structure, evidences of synergic effect. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination and insertion reactions.

#### **Catalysis by Organometallic Compounds (10L)**

Study of the following industrial processes

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Hydroformylation
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Ziegler-Natta catalysis for olefin polymerization.

#### **Reaction Kinetics and Mechanism (12L)**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect and its application in complex synthesis, 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.

#### **Practical**

##### **Qualitative semimicro analysis**

Qualitative semimicro analysis of mixtures containing four radicals. Emphasis should be given to the understanding of the chemistry of different reactions and to assign the most probable composition.

Cation Radicals:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}/\text{Mn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}/\text{Co}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}/\text{Sn}^{4+}$ ,  $\text{As}^{3+}/\text{As}^{5+}$ ,  $\text{Sb}^{3+}/\text{Sb}^{5+}$ ,  $\text{NH}_4^+$ ,  $\text{Mg}^{2+}$ .

Anion Radicals:  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{BrO}_3^-$ ,  $\text{I}^-$ ,  $\text{IO}_3^-$ ,  $\text{SCN}^-$ ,  $\text{S}_2^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CrO}_4^{2-}$  /  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{Fe}(\text{CN})_6^{4-}$ ,  $\text{Fe}(\text{CN})_6^{3-}$ .

Insoluble Materials:  $\text{Al}_2\text{O}_3(\text{ig})$ ,  $\text{Fe}_2\text{O}_3(\text{ig})$ ,  $\text{Cr}_2\text{O}_3(\text{ig})$ ,  $\text{SnO}_2$ ,  $\text{SrSO}_4$ ,  $\text{BaSO}_4$ ,  $\text{CaF}_2$ ,  $\text{PbSO}_4$ .

#### **Title: Physical Chemistry IV**

**Instructor: Mr. Partha Sarathi Mahato**

#### **Molecular Spectroscopy (18L)**

1. Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation
2. Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution
3. 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; Diatomic vibrating rotator, P, Q, R branches
4. 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

#### **Photochemistry (16L)**

1. Lambert-Beer's law: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients; Laws of photochemistry, Stark-Einstein law of photochemical equivalence quantum yield, actinometry, examples of low and high quantum yields
2. Photochemical Processes: Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra; Bond dissociation and principle of determination of dissociation energy (ground state); Decay of excited states by radiative and non-radiative paths; Pre-dissociation; Fluorescence and phosphorescence, Jablonskii diagram;
3. Rate of Photochemical processes: Photochemical equilibrium and the differential rate of photochemical reactions, Photostationary state;  $\text{HI}$  decomposition,  $\text{H}_2$ - $\text{Br}_2$  reaction, dimerisation of anthracene; photosensitised reactions, quenching; Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence

#### **Resonance Spectroscopy: NMR, ESR & Electrical Properties of Molecules (20L)**

1. 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
2. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals



3. Dipole moment and polarizability: Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules; Clausius-Mosotti equation and Debye equation (both without derivation) and their application; Determination of dipole moments

#### **Catalysis (6L)**

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot, turn-over number; Autocatalysis; periodic reactions

#### **Practical**

1. Determination of CMC from surface tension measurements
2. Verification of Beer and Lambert's Law for  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  solution
3. Study of kinetics of  $\text{K}_2\text{S}_2\text{O}_8 + \text{KI}$  reaction, spectrophotometrically
4. Determination of pH of unknown buffer, spectrophotometrically
5. Effect of ionic strength on the rate of Persulphate – Iodide reaction

### **Title: Green Chemistry**

**Instructor: Dr. Soumen Mistri**

#### **Introduction to Green Chemistry (5L)**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/Obstacles in the pursuit of the goals of Green Chemistry

#### **Principles of Green Chemistry and Designing a Chemical synthesis (25L)**

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

1. Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
2. Prevention/ minimization of hazardous/ toxic products reducing toxicity.  
 $\text{risk} = (\text{function}) \text{hazard} \times \text{exposure}$ ; waste or pollution prevention hierarchy.
3. Green solvents—supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
4. Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
5. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.
6. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
7. Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbocarbaryl) and Flixborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
8. Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

#### **Examples of Green Synthesis/ Reactions and some real world cases (22L)**

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
4. Surfactants for carbon dioxide replacing smog producing and ozone depleting solvents with  $\text{CO}_2$  for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.

7. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

8. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils

9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

#### **Future Trends in Green Chemistry (8L)**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

#### **Practical**

##### **Safer starting materials**

1. Preparation and characterization of nanoparticles of gold using tea leaves.

##### **Using renewable resources**

1. Preparation of biodiesel from vegetable/ waste cooking oil.

##### **Avoiding waste**

Principle of atom economy.

1. Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

2. Preparation of propene by two methods can be studied

a. Triethylamine ion + OH- → propene + trimethylpropene + water

b.  $\xrightarrow{\text{H}_2\text{SO}_4/\text{heat}}$  I-propanol → Propene + water

3. Other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

##### **Use of enzymes as catalysts**

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

##### **Alternative Green solvents**

Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice. Mechanochemical solvent free synthesis of azomethines

##### **Alternative sources of energy**

1. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
2. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

#### **Title: Polymer Chemistry**

##### **Introduction and history of polymeric materials(4L)**

**Instructor: Dr. Keshab Mondal**

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers.

##### **Functionality and its importance(4L)**

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bi-functional systems, Poly-functional systems.

##### **Kinetics of Polymerization(6L)**

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.

##### **Crystallization and crystallinity(6L)**

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.

##### **Nature and structure of polymers(3L)**

Structure Property relationships.

##### **Determination of molecular weight of polymers(7L)**

(M<sub>n</sub>, M<sub>w</sub>, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

##### **Glass transition temperature (T<sub>g</sub>) and determination of T<sub>g</sub> (5L)**

Free volume theory, WLF equation, Factors affecting glass transition temperature (T<sub>g</sub>).

##### **Polymer Solution (10 L)**

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.

### **Properties of Polymer (15L)**

(Physical, thermal, Flow & Mechanical Properties)

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 polythiophene)].

### **Practical**

#### **Polymer Synthesis**

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

#### **Polymer characterization**

1. Determination of molecular weight by viscometry:
  - a. Polyacrylamide-aq. NaNO<sub>2</sub> solution
  - b. (Poly vinyl propylidene (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

### **B.Sc Program (Sem VI)**

**Title: Green Chemistry**

**Instructor: Dr. Soumen Mistri**

### **Introduction to Green Chemistry (5L)**

1. What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

### **Principles of Green Chemistry and Designing a Chemical synthesis (25L)**

Twelve principles of Green Chemistry with their explanations and examples and special emphasis on the following:

1. Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products, Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
2. Prevention/ minimization of hazardous/ toxic products reducing toxicity.  
risk = (function) hazard × exposure; waste or pollution prevention hierarchy.
1. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.

2. Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
3. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.
4. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
5. Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbaryl) and Flixborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
6. Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

#### **Examples of Green Synthesis/ Reactions and some real world cases (22L)**

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)

1. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction

3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

1. Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.
2. Designing of Environmentally safe marine antifoulant.
3. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
4. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
5. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils
6. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

#### **Future Trends in Green Chemistry (8L)**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis (C2S3); Green chemistry in sustainable development.

#### **Practical**

##### **Safer starting materials**

1. Preparation and characterization of nanoparticles of gold using tea leaves.

##### **Using renewable resources**

1. Preparation of biodiesel from vegetable/ waste cooking oil.

##### **Avoiding waste**

Principle of atom economy.

1. Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

2. Preparation of propene by two methods can be studied



H<sub>2</sub>SO<sub>4</sub>/heat

b. I-propanol  $\rightarrow$  Propene + water

1. Other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

##### **Use of enzymes as catalysts**

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

##### **Alternative Green solvents**

Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice. Mechanochemical solvent free synthesis of azomethines

##### **Alternative sources of energy**

1. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
2. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.