

**CHOICE BASED CREDIT  
SYSTEM**

**B. SC. HONOURS**

**DEPARTMENT OF CHEMISTRY  
VISVA-BHARATI**

# Course Structure (Chemistry-Major)

## Details of courses under B.Sc. (Honours)

Course	*Credits	
	Theory+ Practical	Theory + Tutorial
<b>I. Core Course</b>		
<b>(14 Papers)</b>	14×4= 56	14×5=70
<b>Core Course Practical / Tutorial*</b>		
<b>(14 Papers)</b>	14×2=28	14×1=14
<b>II. Elective Course</b>		
<b>(8 Papers)</b>		
A.1. Discipline Specific Elective	4×4=16	4×5=20
<b>(4 Papers)</b>		
A.2. Discipline Specific Elective		
Practical/Tutorial*	4×2=8	4×1=4
<b>(4 Papers)</b>		
B.1. Generic Elective/		
Interdisciplinary	4×4=16	4×5=20
<b>(4 Papers)</b>		
B.2. Generic Elective		
Practical/ Tutorial*	4×2=8	4×1=4
<b>(4 Papers)</b>		
<b>Optional Dissertation or project work in place of one Discipline Specific Elective paper (6 credits) in 6<sup>th</sup> Semester</b>		
<b>3. Ability Enhancement Courses</b>		
<b>1. Ability Enhancement Compulsory</b>		
<b>(2 Papers of 2 credit each)</b>	2×2=4	2×2=4
Environmental Science		
English/MIL Communication		
<b>2. Ability Enhancement Elective (Skill Based)</b>		
<b>(Minimum 2)</b>	2×2=4	2×2=4
<b>(2 Papers of 2 credit each)</b>		
<b>Total credit</b>	<b>140</b>	<b>140</b>

\* wherever there is a practical there will be no tutorial and vice-versa

**SCHEME FOR CHOICE BASED CREDIT SYSTEM IN**  
**B. Sc. Honours (Chemistry)**

	<b>CORE COURSE (14)</b>	<b>Ability Enhancement Compulsory Course (AECC) (2)</b>	<b>Ability Enhancement Elective Course (AEEC) (2) (Skill Based)</b>	<b>Elective: Discipline Specific DSE (4)</b>	<b>Elective: Generic (GE) (4)</b>
I	CC-1: Inorganic Chemistry (4+2)	(English Communication/MIL) /Environmental Science			GEC-1
	CC2: Group-A: Organic Chemistry (2+1), Group-B: Physical Chemistry (3)				
II	CC3 Group-A: Inorganic Chemistry (2+1), Group-B: Physical Chemistry (3)	Environmental Science/(English/MIL Communication)			GEC-2
	CC4: Organic Chemistry (4+2)				
III	CC5: Inorganic Chemistry (4+2)		SEC -1		GEC-3
	CC6: Organic Chemistry (4+2)				
	CC7: Physical Chemistry (5+1)				
IV	CC8: Inorganic Chemistry (4+2)		SEC -2		GEC-4
	CC9: Organic Chemistry (4+2)				
	CC10: Physical Chemistry (5+1)				
V	CC11 Group-A: Inorganic Chemistry (3), Group-B: Organic Chemistry (2+1)			DSE-1	
	CC12: Physical Chemistry (4+2)			DSE -2	
VI	CC13 Group-A: Inorganic Chemistry (2+1), Group-B: Organic Chemistry (3)			DSE -3	
	CC14: Physical Chemistry (4+2)			DSE -4	

## Semester I

### **CHEMISTRY-CC1:**

### **Inorganic Chemistry**

### **Group A (Theory, Credits: -04) (60 Lectures)**

**Atomic Structure:** Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of  $s$ ,  $p$ ,  $d$  and  $f$  orbitals. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number. **(14 Lectures)**

**Periodicity of Elements:**  $s$ ,  $p$ ,  $d$ ,  $f$  block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to  $s$  and  $p$ -block. (a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table. (b) Atomic radii (van der Waals) (c) Ionic and crystal radii. (d) Covalent radii (octahedral and tetrahedral) (e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy. (f) Electron gain enthalpy, trends of electron gain enthalpy. (g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio. **(16 Lectures)**

### **Chemical Bonding:**

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules  $N_2$ ,  $O_2$ ,  $C_2$ ,  $B_2$ ,  $F_2$ ,  $CO$ ,  $NO$ , and their ions;  $HCl$ ,  $BeF_2$ ,  $CO_2$ , (idea of  $s$ - $p$  mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ( $\pi$  and  $\sigma$  bond approach) and bond lengths. Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(iv) *Weak Chemical Forces:* van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process. **(26 Lectures)**

**Oxidation-Reduction-1:** Redox equations. Nernst equation (without derivation). Influences of complex formation, precipitation and change of pH on Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class. **(4 Lectures)**

## **Group B (Practical, Credits: -02) (60 Lectures)**

### **(A) Titrimetric Analysis**

(i) Calibration and use of apparatus (ii) Preparation of solutions of different Molarity/Normality of titrants

### **(B) Acid-Base Titrations**

(i) Estimation of carbonate and hydroxide present together in mixture. (ii) Estimation of carbonate and bicarbonate present together in a mixture. (iii) Estimation of free alkali present in different soaps/detergents

### **(C) Oxidation-Reduction Titrimetry**

(i) Estimation of Fe(II) and oxalic acid using standardized  $\text{KMnO}_4$  solution. (ii) Estimation of oxalic acid and sodium oxalate in a given mixture. (iii) Estimation of Fe(II) with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal (diphenylamine, anthranilic acid) and external indicator.

### **(D) Inorganic preparations-1**

(i) Cuprous Chloride,  $\text{Cu}_2\text{Cl}_2$  (ii) Preparation of Manganese(III) phosphate,  $\text{MnPO}_4 \cdot \text{H}_2\text{O}$  (iii) Preparation of Aluminium potassium sulphate  $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$  (Potash alum) or Chrome alum.

## **CHEMISTRY-CC2:**

### **Group A (Theory, Organic Chemistry)**

**Credit 2 + 1 (Tutorial) ; Lecture 30 +15**

#### **Basics of Organic Chemistry:**

**12 Lectures**

*Organic Compounds:* Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties.

*Electronic Displacements:* Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids and bases; their relative strength.

Homolytic and Heterolytic fission with suitable examples; Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Nucleophilicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes.

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

**Stereochemistry:****18 Lectures**

Concept of constitution, configuration and conformation of Organic molecules, Geometrical isomerism, enantiomerism and diastereomerism, chirality and optical activity, elements of symmetry, asymmetry and dissymmetry, R/S, E/Z, D/L, syn/anti, cis/trans, meso/dl, threo/erythro –nomenclature system, Fischer, Sawhorse, Flying Wedg, Newman formulae, Racemization and resolution, resolution of racemic acids, bases and alcohols; optical purity/enantiomeric excess. Axial chirality of allenes, biphenyls, conformation of cyclohexane systems, Topicity of ligands and faces (elementary idea); homotopic, enantiotopic and diastereotopic ligands and faces, prochirality, pro-R/Pro-S and re/si descriptors, Conformational isomerism – eclipsed, staggered gauche and anti; concept of dihedral and torsion angle, energy diagram during variation of torsion angle.

**Group B (Theory, Physical Chemistry)****Credit 3 ; Lecture 45****Gaseous state: (22 L)**

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities. collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of  $\lambda$  from  $\eta$ ; variation of viscosity with temperature and pressure. Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

**Zeroth & 1st Laws of Thermodynamics****(13 L)**

Motivation of study of thermodynamics, Important vocabularies of thermodynamics, isolated, closed and open systems, thermodynamic equilibrium state. state and path functions, Realization of existence of a state variable temperature from thermal equilibrium (zeroth law of thermodynamics). Definition of work and Heat. Reversible and irreversible processes. 1st law of thermodynamics and realization of existence of a state variable (internal energy, E). Intensive and extensive variables, Properties of internal energy. Ordinary derivative, partial derivative, cyclic rule, exact differential. Determination of  $(\partial E / \partial V)_T$ . experiments of Jules and Years. Realization of existence of another state variable, Enthalpy. Relation between CP and CV. Adiabatic process. calculations of q, w, and H for reversible, irreversible and free expansion of gases (ideal and change of U and  $\eta$  van der Waals) under isothermal and adiabatic conditions.

**Thermochemistry****( 10 L)**

Heats of reactions: Law of Lavoisier & Laplace, Hess's Law and its usefulness ,standard states; enthalpy of formation of molecules and ions, standard enthalpy of formation other than 298.15 K, enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reaction and energys. Adiabatic flame temperature, explosion temperature., limitation of bond energy,

crystal energy, salvation energy. Heat of neutralization Relation between heat of reaction at constant volume and pressure respectively. Calorimetric measurement of enthalpy of reaction.

## **Semester II**

### **CHEMISTRY-CC3:**

#### **Group A (Theory, Inorganic Chemistry)**

**(Credits: Theory-02; Tutorial-01)**

**Theory: 30 Lectures; Tutorial: 15 hours**

#### **Oxidation-Reduction-II:**

Formal potential, Stability of various oxidation states and e.m.f. diagrams (Latimer, Frost and Pourbaix) of common elements; **(7 Lectures)**

#### **Radioactivity:**

Nuclear stability and nuclear binding energy, Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes. Radio-chemical method: Principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures. **(15 Lectures).**

#### **Coordination Chemistry-1:**

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. **(8 Lectures)**

#### **Group B (Theory, Physical Chemistry)**

**Credit 3; Lecture 45**

#### **Chemical Kinetics (20 L)**

Definition of mole reaction and advancement of chemical reaction, Definition of velocity of chemical reaction in terms of advancement of chemical reaction, Rate law of chemical reaction at constant volume. Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Study of fast reaction in solution flow method, relaxation method Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, absolute rate theory, uni-molecular reaction, Lindemann mechanism. Introduction of concept of reaction coordinate and potential energy surface for very simple reaction.

#### **2nd Law of Thermodynamics**

**(25 L)**

Natural and unnatural process, Limitation of the first law of thermodynamic, statements of the second law

and their equivalence, Existence of direction of change and arrow of time for the thermodynamic system, Searching of a state property to determine the criteria of spontaneous change. Carnot cycle, consistency of the cycle with the 1st law, efficiency of an heat engine, efficiency of both reversible and irreversible engines. Development of thermodynamic scale of temperature and relation with other scales., Definition of entropy, Calculation of entropy change for reversible and irreversible processes. Thermodynamic interpretation of entropy. Clausius inequality, Qualitative correlation between entropy and spontaneity for transformation of an isolated system, definition of micro state. Interpretation of entropy based on phase space. Entropy change for phase change, Determination of interaction energy in liquid and solid, Trouton's rule and its modification. Dependence of entropy on the other state variable.

## **CHEMISTRY-CC4: Organic Chemistry**

### **Group A (Theory, Credits: -04) (60 Lectures)**

#### **Chemistry of Aliphatic Hydrocarbons:**

#### **Lecture 20**

##### **A. Carbon-Carbon sigma bonds**

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity.

##### **B. Carbon-Carbon pi bonds:**

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

*Reactions of alkenes:* Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

*Reactions of alkynes:* Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

#### **Alkanes, Cycloalkanes and Conformational Analysis:**

#### **16 Lectures**

Nomenclature, types of strain, Bayer strain theory, measurement of strain and classification of ring sizes, consequences of strain in small, normal, medium and large ring, conformation behaviours of normal rings, substituted cyclohexanes, effect of substitution on ring conformation of cyclohexane, conformation of cyclohexene, effect of strain on reactivity, ring synthesis - principles controlling ring closure reactions, rules for ring closure (Baldwin's rule), ring expansion and contraction processes, polycyclic system - Bredt's rule, Conformational analysis of n-butane, dihaloethanes, glycols.

#### **Aromatic Hydrocarbons:**

#### **12 Lectures**

*Aromaticity:* Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and



heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

### **Chemistry of Halogenated Hydrocarbons:**

**12 Lecture**

*Alkyl halides:* Methods of preparation, nucleophilic substitution reactions –  $S_N1$ ,  $S_N2$  and  $S_Ni$  mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

*Aryl halides:* Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution;  $S_NAr$ , Benzyne mechanism. Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

### **Group B (Practical, Credits: -02) (60 Lectures)**

1. Purification of organic compounds by crystallization using the following solvents:
  - a. Water
  - b. Alcohol
  - c. Alcohol-Water
2. Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
3. Qualitative analysis of solid organic compounds in respect of the following: Detection of elements, determination of M.P., detection of functional group and preparation of a derivative (with M.P.):
4. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.

## **Semester III**

### **CHEMISTRY- CC5: Inorganic Chemistry**

#### **GROUP A (Theory)**

**(Credits: Theory-04) Theory: 60 Lectures**

**General Principles of Metallurgy:** 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. **(6 Lectures)**

**Acids and Bases:** Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, leveling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle. Acid-Base equilibria in solution: Hydrolysis of salts, pH calculation. Buffer.

**(8 Lectures)**

**Chemistry of *s* and *p* Block Elements:** Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements. Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens. **(30 Lectures)**

**Noble Gases:** 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  $\text{XeF}_2$ ). Molecular shapes of noble gas compounds (VSEPR theory). **(8 Lectures)**

**Inorganic Polymers:** Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates. **(8 Lectures)**

**GROUP B (practical)**  
**Credit point-02 - 60 lectures**

**(A) Iodo / Iodimetric Titrations**

- (i) Estimation of Cu(II) and  $\text{K}_2\text{Cr}_2\text{O}_7$  using sodium thiosulphate solution (Iodimetrically).
- (ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
- (iii) Estimation of available chlorine in bleaching powder iodometrically.

**(B) Gravimetric Analysis:**

- i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
- ii. Estimation of copper as  $\text{CuSCN}$
- iii. Estimation of iron as  $\text{Fe}_2\text{O}_3$  by precipitating iron as  $\text{Fe}(\text{OH})_3$ .
- iv. Estimation of Al (III) by precipitating with oxine and weighing as  $\text{Al}(\text{oxine})_3$  (aluminium oxinate).

**(C) Inorganic Preparations-II:**

- i. Tetraamminecopper (II) sulphate,  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$
- ii. Cis and trans  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2 \cdot (\text{H}_2\text{O})_2]$ , Potassium dioxalatodiaquachromate (III)

iii. Tetraamminecarbonatocobalt (III) ion

iv. Potassium tris(oxalate)ferrate(III)

#### **(D) Chromatography of metal ions:**

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

- i. Ni (II) and Co (II)
- ii. Fe (III) and Al (III)

### **CHEMISTRY- CC6: Organic Chemistry Credit 4 +2 (Practical); Lecture 60 +60**

#### **GROUP A (Theory)**

##### **Alcohols, Phenols, Ethers and Epoxides:**

**8 Lectures**

*Alcohols:* preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement.

*Phenols:* Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe’s–Schmidt Reactions, Fries and Claisen rearrangements with mechanism.

*Ethers and Epoxides:* Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and  $\text{LiAlH}_4$

##### **Carbonyl Compounds:**

**20 Lectures**

Structure, reactivity and preparation; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, -substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner,  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , MPV, PDC and PGC);

Addition reactions of unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

##### **Carboxylic Acids and their Derivatives:**

**10 Lectures**

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids;

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmannbromamide degradation and Curtius rearrangement.

### **Nitrogen and Sulphur containing compounds:**

**10 Lectures**

Preparation and important reactions of nitro and compounds, nitriles and isonitriles Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid.

Diazonium Salts: Preparation and their synthetic applications.

Preparation and reactions of thiols, thioethers and sulphonic acids.

### **Organometallic compounds of Mg, Li, Cu, B, Si:**

**12 Lectures**

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.

### **GROUP B (Practical)**

#### **Practical Organic Chemistry: Credit: 2: 60 Lecture**

1. Identification with general reaction and tests of the following compounds

- |                   |                  |                  |                   |
|-------------------|------------------|------------------|-------------------|
| a) Methyl alcohol | b) Ethyl alcohol | c) Glycerol      | d) Acetone        |
| e) Formic acid    | f) Acetic acid   | g) Aniline       | h) Nitrobenzene   |
| i) Benzyl alcohol | j) Tartaric acid | k) Succinic acid | l) Salicylic acid |
| m) Cane sugar     | n) Glucose       | m) Resorcinol    |                   |

### **CHEMISTRY- CC7:**

#### **PHYSICAL CHEMISTRY-III (Credits: Theory-05, Tutorial-01)**

**Theory: 75 Lectures, Tutorial- 15 hours**

#### **Extension of the second law : (8 Lectures)**

Condition of spontaneity & equilibrium. Thermochemical equation of state. , definition of G and A, variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson

coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

**Third Law:** *Nernst heat theorem and its consequences*, Statement of third law and its experimental verification, concept of residual entropy, calculation of absolute entropy of molecules. (4Lectures)

### **Systems of Variable Composition:**

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. (8 Lectures)

### **Thermodynamics of reaction vessel :**

Criteria of thermodynamic equilibrium, degree of advancement of a reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants  $K_p$ ,  $K_c$  and  $K_x$ . Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase. (13 Lectures)

### **Liquid state: (9L)**

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure, coefficient of viscosity, and their determination. laminar flow, turbulent flow, Reynolds number, Poiseuille's law, Effect of addition of various solutes on viscosity. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water. Diffusion, Fick's law of diffusion, diffusion coefficient

### **Conductance**

Arrhenius theory of electrolytic dissociation. Application of Ohm's law to electrolytic solution, Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules. Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts. (13 Lectures)

### **Quantum Mechanics –I (20 Lectures)**

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

## Semester IV

### **CHEMISTRY-CC8:**

### **INORGANIC CHEMISTRY-IV**

### **GROUP-A (theory)**

**(Credits: Theory-04) Theory: 60 Lectures**

#### **Coordination Chemistry-II:**

Valence bond theory (inner and outer orbital complexes) and its limitations. Electroneutrality principle and back bonding. Crystal field theory, measurement of  $10 Dq$  ( $\Delta_o$ ), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of  $10 Dq$  ( $\Delta_o$ ,  $\Delta_t$ ). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry: Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

Magnetism and colour: Orbital and spin magnetic moments, spin only moments of  $d^n$  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. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea) **(26 Lectures)**

#### **Transition Elements:**

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stabilization of high and low oxidation states with designed systems. Stability of various oxidation states. Difference between the first, second and third transition series. Chemistry of Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Cu in various oxidation states and magneto-structural correlations in specific cases (excluding their metallurgy) **(18 Lectures)**

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

Electronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). **(6 Lectures)**

#### **Theoretical Principles in Qualitative Analysis ( $H_2S$ Scheme)**

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II. **(10 Lectures)**

### **GROUP -B**

### **Inorganic Chemistry PRACTICAL**

**60 Lectures (Credit: Practical: 02)**

#### **(A) Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations:**

Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:  $CO_3^{2-}$ ,  $NO_2^-$ ,  $S^{2-}$ ,  $SO_3^{2-}$ ,  $S_2O_3^{2-}$ ,  $CH_3COO^-$ ,  $F^-$ ,  $Cl^-$ ,  $Br^-$ ,  $I^-$ ,  $NO_3^-$ ,

$\text{BO}_3^{3-}$ ,  $\text{C}_2\text{O}_4^{2-}$ ,  $\text{PO}_4^{3-}$ ,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Pb}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}$ ,  $\text{Sb}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$

Mixtures should preferably contain one interfering anion, **or** insoluble component ( $\text{BaSO}_4$ ,  $\text{SrSO}_4$ ,  $\text{PbSO}_4$ ,  $\text{CaF}_2$  or  $\text{Al}_2\text{O}_3$ ) **or** combination of anions e.g.  $\text{CO}_3^{2-}$  and  $\text{SO}_3^{2-}$ ,  $\text{NO}_2^-$  and  $\text{NO}_3^-$ ,  $\text{Cl}^-$  and  $\text{Br}^-$ ,  $\text{Cl}^-$  and  $\text{I}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ,  $\text{NO}_3^-$  and  $\text{Br}^-$ ,  $\text{NO}_3^-$  and  $\text{I}^-$ .

Spot tests should be done whenever possible.

### **(B) Some experiments**

- Measurement of 10 Dq by spectrophotometric method
- Verification of spectrochemical series.
- Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.
- Preparation of acetylacetonato complexes of  $\text{Cu}^{2+}/\text{Fe}^{3+}$ . Find the  $\lambda_{\text{max}}$  of the complex.
- Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

## **CHEMISTRY-CC9:**

### **ORGANIC CHEMISTRY-IV**

#### **Credit 4 +2 (Tutorial): Lecture 60 +60**

#### **GROUP-A Theory (credit: 4, 60 lectures)**

##### **Dynamic Stereochemistry of acyclic and cyclic compounds:**

##### **14 Lecture**

Conformation, reactivity and mechanism of acyclic and cyclic systems, Asymmetric synthesis and asymmetric induction, Acyclic stereoselection, Addition of nucleophiles to carbonyl compounds: 1,2-asymmetric induction, Cram's open chain, cyclic(chelate) and dipolar model, Prelog's rule. The aldol reaction. Neighbouring group participation and molecular rearrangements.

Conformation and reactivity of alicyclic compounds, effect of substituent stereochemistry on reactivity of cyclohexane derivatives, steric effect, stereoelectronic effects, reduction of cyclic ketones and reaction of cyclic epoxides, neighbouring group effects, effect of conformation on rearrangement and transannular reactions in alicyclic system, lactonization reactions of cyclohexane systems, oxidation of cyclohexanols with chromic acid, steric assistance and steric hindrance. Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones, formation of axial and equatorial alcohols.

##### **Heterocyclic Compounds:**

##### **12 Lectures**

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup

synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch Reaction; Derivatives of furan: Furfural and furoic acid.

### **Alkaloids & Terpenes:**

**6 Lectures**

Natural occurrence, General structural features, Isolation and their physiological action Hoffmann's exhaustive methylation, Emde's modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine.

Occurrence, classification, isoprene rule; Elucidation of structure and synthesis of Citral, Neral and -terpineol.

### **Carbohydrates:**

**12 Lectures**

Occurrence, classification and their biological importance.

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani- Fischer synthesis and Ruff degradation;

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

### **Polynuclear Hydrocarbons:**

**8 Lectures**

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons.

### **Amino Acids, Peptides and Proteins:**

**8 Lecture**

Amino acids, Peptides and their classification. -Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis;

Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups -Solid-phase synthesis

## **GROUP-B Practical (credit: 2, 60 lectures)**

### **Practical**

1. Organic preparations:

i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and phenols ( *n*-naphthol, vanillin, salicylic acid) by any one method:

a. Using conventional method.

b. Using green approach

ii. Benzoylation of one of the following amines (aniline, *o*-, *m*-, *p*-toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols ( *n*-naphthol, resorcinol, *p*-cresol) by Schotten-Baumann reaction.

iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).

iv. Bromination of any one of the following:



- a. Acetanilide by conventional methods
  - b. Acetanilide using green approach (Bromate-bromide method)
  - v. Nitration of any one of the following:
    - a. Acetanilide/nitrobenzene by conventional method
    - b. Salicylic acid by green approach (using ceric ammonium nitrate).
  - vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
  - vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
  - viii. Hydrolysis of amides and esters.
  - ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
  - x. *S*-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
  - xi. Aldol condensation using either conventional or green method.
  - xii. Benzil-Benzilic acid rearrangement.
2. Extraction of caffeine from tea leaves.

## **CHEMISTRY- CC10:**

### **PHYSICAL CHEMISTRY-IV**

**(Credits: Theory-05, Tutorial -01) Theory: 75 Lectures**

#### **Solutions and Colligative Properties: (9 Lectures)**

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions. 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.

#### **Phase Equilibria: (23 Lectures)**

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius- Clapeyron equation and its applications to solidliquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions. Three component systems, water- chloroform-acetic acid system, triangular plots. *Binary solutions*: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications.)

#### **Electrochemistry (23 Lectures)**

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. Electrostatics, electrochemical system, thermodynamics of electro chemical systems, understanding and setup of criteria of conversion of chemical energy into electrical energy, Galvanic cells and their thermodynamics, Chemical concentration 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 Debye-Huckel limiting law and its application to (i) Determination of Standard EMF , (ii) ionic reactions to account salt effect, Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb<sub>2</sub>O<sub>3</sub> electrodes. Formal potential and its importance. 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).)

## **Quantum Mechanics –II**

**(20 Lectures)**

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution. 32 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.

## **Semester V**

### **CHEMISTRY-CC11:**

#### **GROUP- A (Theory)**

#### **INORGANIC CHEMISTRY-V**

**(Credits: Theory-03,) Theory: 45 Lectures,**

#### **Bioinorganic Chemistry:**

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

Important metal complexes in medicine (examples only), antimicrobial activity, antiarthritic gold complexes, anticancer compounds (Pt-complexes and metallocenes), lithium therapy in psychiatric mind disorder **(22 Lectures)**

#### **Reaction Kinetics and Mechanism**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans-effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes. **(23 Lectures)**

#### **GROUP –B (theory)**

#### **ORGANIC CHEMISTRY- ,**

**Credit 2 + 1 (Tutorial) : lecture 30 +15**

#### **Organic Spectroscopy:**

**20 Lectures**

General principles Introduction to absorption and emission spectroscopy.

*UV Spectroscopy:* Types of electronic transitions,  $\lambda_{\text{max}}$ , Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of  $\lambda_{\text{max}}$  for the following systems:  $\alpha,\beta$ -unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

*IR Spectroscopy:* Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

*NMR Spectroscopy:* Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds.

Applications of IR, UV and NMR for identification of simple organic molecules.

Elementary idea on mass spectrometry.

## **Dyes:**

**5 Lectures**

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; Synthesis and applications of: Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein; Natural dyes –structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

## **Polymers:**

**5 Lectures**

Introduction and classification including di-block, tri-block and amphiphilic polymers; Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions -Addition and condensation -Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes; Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics – natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives; Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples.

**CHEMISTRY- CC12:**

**PHYSICAL CHEMISTRY V**

**GROUP-A (Theory)**

**(Credits: Theory-04) Theory: 60 Lectures**

## **Quantum Chemistry:**

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle- in-a-box, harmonic oscillator, hydrogen atom). Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of  $H_2$  +. Bonding and antibonding orbitals. Qualitative extension to  $H_2$ . Comparison of LCAO-MO and VB treatments of  $H_2$  (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic ( $BeH_2$ ,  $H_2O$ ) molecules. Qualitative MO theory and its application to  $AH_2$  type molecules. **(15 Lectures)**

## **Surface chemistry and catalysis (12 Lectures)**

Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state, BET equation with its derivation surface tension and its determination. Gibbs adsorption isotherm, Effect of addition of various solutes on surface tension. Explanation of cleansing action of detergents.

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

## **Ionic equilibria:**

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment). Salt hydrolysis- calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations. Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants. **(13 Lectures)**

## **Molecular Spectroscopy:**

Interaction of electromagnetic radiation with molecules and various types of spectra; Born- Oppenheimer approximation. Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution. Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches. Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. **(20 Lectures)**

## **GROUP -B**

### **PHYSICAL CHEMISTRY PRACTICAL-**

**60 Lectures (6 hours per week), Credits: -02**

**1. Surface tension measurements.**

a. Determine the surface tension by (i) drop number (ii) drop weight method. b. Study the variation of surface tension of detergent solutions with concentration.

**4. Viscosity measurement using Ostwald's viscometer.** a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.

b. Study the variation of viscosity of sucrose solution with the concentration of solute.

**5. Indexing of a given powder diffraction pattern of a cubic crystalline system.**

**6. pH metry**

a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.

b. Preparation of buffer solutions of different pH

i. Sodium acetate-acetic acid

ii. Ammonium chloride-ammonium hydroxide

c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.

d. Determination of dissociation constant of a weak acid.

**Conductometry**

I. Determination of cell constant

II. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid. III. Perform the following conductometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. Mixture of strong acid and weak acid vs. strong base

iv. Strong acid vs. weak base

**Kinetics**

V. Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction

2. Integrated rate method: a. Acid hydrolysis of methyl acetate with hydrochloric acid. b. Saponification of ethyl acetate.

3. Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate.

## **Semester VI**

**CHEMISTRY-CC13:**

**GROUP-A (Theory)**

**INORGANIC CHEMISTRY**

**(Credits: Theory-02, Tutorial-01) Theory: 30 Lectures, Tutorial-15 hours**

**Organometallic Compounds**

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT.  $\pi$ -acceptor behaviour of CO (MO diagram of CO to be discussed),

synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls. Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene. **(20 Lectures)**

### **Catalysis by Organometallic Compounds**

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinsons Catalyst)
2. Hydroformylation (Co salts)
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Synthesis gas by metal carbonyl complexes **(10 Lectures)**

## **GROUP –B (Theory)**

### **ORGANIC CHEMISTRY**

#### **Credit 3: Lecture 45**

### **Pericyclic Reactions:**

**Lecture 12**

Mechanism, stereochemistry, regioselectivity in case of

*Electrocyclic reactions:* FMO approach involving 4 - and 6 -electrons (thermal and photochemical) and corresponding cycloreversion reactions.

*Cycloaddition reactions:* FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.

*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.

### **Retrosynthetic analysis and functional group interconversion**

**12 Lecture**

Basic concept on retrosynthesis, disconnection approach towards synthesis of bifunctional molecules (both cyclic and acyclic), concept of synthons, synthetic equivalents, functional group interconversion, Protection and deprotection of common functional groups in synthetic route, activation of synthetic equivalents, Disconnection and synthesis of (1,3),(1,4) and (1,5)-dioxxygenated compounds, Some specific examples indicating the retrosynthetic approach to design a total synthesis.

### **Nucleic Acids, Enzymes and Lipids**

**12 Lectures**

Components of nucleic acids, Nucleosides and nucleotides;

Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine;

Structure of polynucleotides.

Introduction, classification and characteristics of enzymes. Salient features of active site of

enzymes. Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition). Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

## **Concept of Energy in Biosystems and Pharmaceutical Compounds**

**9 Lectures**

Cells obtain energy by the oxidation of foodstuff (organic molecules).

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change.

Agents for transfer of electrons in biological redox systems: NAD<sup>+</sup>, FAD.

Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate.

Caloric value of food, standard caloric content of food types.

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

## **CHEMISTRY- CC14:**

### **PHYSICAL CHEMISTRY**

#### **GROUP- A (Theory)**

**Credits: Theory-04) Theory: 60 Lectures**

### **Electrical & Magnetic Properties of Atoms and Molecules**

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetismparamagnetism, magnetic susceptibility and its measurement, molecular interpretation.

**(10 Lectures)**

### **Solid state:**

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Scattering of X-rays from a unit cell, Bragg's law, a simple account of rotating crystal method and powder pattern method. Structure factor, missing reflections, Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals. (15 Lectures)

### **Spectroscopy**

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions

of polyenes using free electron model. Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

**(20 Lectures)**

### **Photochemistry**

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, Stern-Volmer Plot, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

**(15 Lectures)**

### **GROUP-B**

#### **PHYSICAL CHEMISTRY PRACTICAL**

**Credits: -02, 60 Lectures**

#### **UV/Visible spectroscopy**

I. Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J molecule}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).

II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .

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

#### **Colourimetry**

I. Verify Lambert-Beer's law and determine the concentration of  $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration.

II. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture.

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

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

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

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

VII. Analysis of the given vibration-rotation spectrum of  $\text{HCl(g)}$ .

#### **Potentiometry**

I Perform the following potentiometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. Dibasic acid vs. strong base

iv. Potassium dichromate vs. Mohr's salt

#### **Phase equilibrium**

I. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.

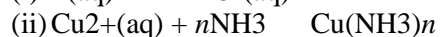
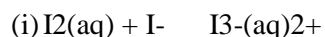
II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:



a. simple eutectic and b. congruently melting systems.

III. Distribution of acetic/ benzoic acid between water and cyclohexane.

IV. Study the equilibrium of at least one of the following reactions by the distribution method:



### Adsorption

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

## Generic Elective Papers (GE) (Minor-Chemistry) for other Departments/ Disciplines: (Credit: 06 each)

### GEC-1: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

#### Section A: Inorganic Chemistry-1 (30 Periods)

**Atomic Structure:** Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of  $r$  and  $r^2$ , Schrodinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers  $m_l$  and  $m_s$ . Shapes of s, p and d atomic orbitals, nodal planes. Discovery of spin, spin quantum number ( $s$ ) and magnetic spin quantum number ( $m_s$ ).

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

(14 Lectures)

#### Chemical Bonding and Molecular Structure

**Ionic Bonding:** General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

**Covalent bonding:** VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of resonance and resonating structures in various inorganic and organic compounds. MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO<sup>+</sup>. Comparison of VB and MO approaches.

**(16 Lectures)**

## **Section B: Organic Chemistry-1 (30 Periods)**

### **Fundamentals of Organic Chemistry**

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Huckel's rule.

**(8 Lectures)**

### **Stereochemistry**

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Three and erythro; D and L; cis – trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

**(10 Lectures)**

### **Aliphatic Hydrocarbons**

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Alkanes: (Upto 5 Carbons). Preparation: Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: Free radical Substitution: Halogenation.

Alkenes: (Upto 5 Carbons) Preparation: Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alk. KMnO<sub>4</sub>) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration—demercuration, Hydroboration—oxidation.

Alkynes: (Upto 5 Carbons) Preparation: Acetylene from CaC<sub>2</sub> and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides.

Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO<sub>4</sub>, ozonolysis and oxidation with hot alk. KMnO<sub>4</sub>.

**(12 Lectures)**

### **GEC-1 LAB: 60 Lectures**

#### **Inorganic Chemistry -**

1. Acidimetry and Alkalimetry,

2. Oxidation and Reduction Methods of Volumetric Analysis with Potassium Permanganate, Potassium Dichromate
3. Iodometry.

**GEC-2: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY-I**  
(Credits: Theory-04, Practicals-02)

**Theory: 60 Lectures**

**Section A: Physical Chemistry-1 (30 Lectures)**

**Chemical Energetics**

Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature — Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

**(10 Lectures)**

**Chemical Equilibrium:**

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between  $\Delta G$  and  $\Delta G^\circ$ , Le Chatelier's principle. Relationships between  $K_p$ ,  $K_c$ , and  $K$ , for reactions involving ideal gases.

**(8 Lectures)**

**Ionic Equilibria:**

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts — applications of solubility product principle.

**(12 Lectures)**

**Section B: Organic Chemistry-2 (30 Lectures)**

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

**Aromatic hydrocarbons**

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel—Crafts' reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

**(8 Lectures)**

**Alkyl and Aryl Halides**

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (SN1, SN2 and SNi) reactions.

Preparation: from alkenes and alcohols.

Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution.

Aryl Halides Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions.

Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by —OH group) and effect of nitro substituent. Benzyne Mechanism:  $\text{KNH}_2/\text{NH}_3$  (or  $\text{NaNH}_2/\text{NH}_3$ ).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

**(8 Lectures)**

### **Alcohols, Phenols and Ethers (Upto 5 Carbons)**

Alcohols: Preparation: Preparation of 1°, 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters.

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk.  $\text{KMnO}_4$ , acidic dichromate, conc.  $\text{HNO}_3$ ). Oppeneauer oxidation Diols: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Phenols: (Phenol case) Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben—Hoesch Condensation, Schotten —Baumann Reaction.

Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehyde, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and from nitriles.

Reactions — Reaction with HCN, ROH,  $\text{NaHSO}_3$ ,  $\text{NH}_2\text{-G}$  derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein—Ponndorf Verley reduction.

**(14 Lectures)**

### **GEC-2 LAB: 60 Lectures**

#### **Organic Chemistry**

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

### **GEC-3: SOLUTIONS, PHASE EQUILIBRIA, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY-II** **(Credits: Theory-06, 90 Lectures)**

#### **Section A: Physical Chemistry-2 (45 Lectures)**

##### **Solutions**

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law — non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids— Principle of steam distillation. Nemst distribution law and its applications, solvent extraction.

**(12 Lectures)**

### **Phase Equilibria**

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius — Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, FeCl<sub>3</sub>-H<sub>2</sub>O and Na— K only).

**(12 Lectures)**

### **Conductance**

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

**(9 Lectures)**

### **Electrochemistry**

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nemst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties:  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  from EMF data. Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).

**(12 Lectures)**

## **Section B: Organic Chemistry-3 (45 Lectures)**

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Carboxylic acids and their derivatives Carboxylic acids (aliphatic and aromatic) Preparation: Acidic and Alkaline hydrolysis of esters. Reactions: Hell — Vohlard - Zelinsky Reaction.

Carboxylic acid derivatives (aliphatic): (Upto 5 carbons)

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion. Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

**(11 Lectures)**

### **Amines and Diazonium Salts**

Amines (Aliphatic and Aromatic): (Upto 5 carbons)

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO<sub>2</sub>, Schotten — Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation. Diazonium salts: Preparation: from aromatic amines. Reactions: conversion to benzene, phenol, dyes.

**(10 Lectures)**

**Amino Acids, Peptides and Proteins:**

Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: ester of  $\text{—COOH}$  group, acetylation of  $\text{—NH}_2$  group, complexation with  $\text{Cu}^{2+}$  ions, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid-phase synthesis.

**(12 Lectures)**

**Carbohydrates:** Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (starch and cellulose) excluding their structure elucidation.

**(12 Lectures)**

**GEC-4: TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS**

**(Credits: Theory-06, 90 Lectures)**

**Section A: Inorganic Chemistry-2 (45 Lectures)**

**Transition Elements (3d series)**

General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

**(18 Lectures)**

**Coordination Chemistry**

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT. IUPAC system of nomenclature.

**(12 Lectures)**

**Crystal Field Theory**

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for Oh and Ti complexes, Tetragonal distortion of octahedral geometry. Jahn—Teller distortion, Square planar coordination.

**(15 Lectures)**

**Section B: Physical Chemistry-3 (45 Lectures)**

**Kinetic Theory of Gases**

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation. Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO<sub>2</sub>.

Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation — derivation not required) and their importance. Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation). Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

**(12 Lectures)**

**Liquids**

Surface tension and its determination using stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

**(9 Lectures)**

**Solids**

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X-Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glasses and liquid crystals.

**(12 Lectures)**

**Chemical Kinetics**

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half-life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).

**(12 Lectures)**

**CHEMISTRY-DSE I-IV (ELECTIVES)****CHEMISTRY-DSE: INORGANIC SPECIALTY POLYMERS(DSE 1)**

**(Credits: Theory-05; Tutorial-01);**

**Theory: 75 Lectures, Tutorial-15 h**

**Introduction:** Types of inorganic polymers, comparison with organic polymers, importance of inorganic polymers, inorganic polymers in biological systems, inorganic chains-homo and hetero catenation (5L)

**General methods of synthesis:** Heat and beat method, co-precipitation method, sol-gel method, hydrothermal method, Step-growth polymerization, chain-growth polymerization, ring-opening polymerization (10L)

**Inorganic polymers of technological importance:** Synthesis, structural aspects and applications: Silicones and siloxanes (silicone grease, oil and rubber), silicates (1D, 2D and 3D), comparison between silicones and silicates; phosphate, superphosphate and polyphosphate (including fertilizers); borazine and polyborazylene (as a ceramic materials), phohazene and polyphosphazene (inorganic rubber) (biomedical relevance), ion-exchange resin (softening of water), inorganic liquid crystal polymer (20L)

**Coordination polymers:** Coordination polymer versus metal organic framework (MOF), natural and synthetic coordination polymers, polymetal clusters, cyano complexes of various metals, specialty of coordination polymers and their utility (10L)

**Polyoxometalates (POM):** Isopolyanions and heteropolyanions, Framework, pH dependent network and degree of polmerization, Role of POM as a catalyst and initiators, Polyoxometalates active against Tumors, Viruses, and Bacteria (10L)

**Conducting polymers:** Introduction, conduction mechanism, difference from metallic conduction, one dimensional conductor (metal), polyacetylene, polyparaphenylene, polyaniline and polypyrrole, water soluble conjugate polymers (pdots), application of conducting polymers (10L)

**Supramolecular polymer:** Properties of supramolecular polymers: Self-healing, optoelectronic and biocompatibility. Hydrogen bonding-based self-healing supramolecular polymers, - interaction-based self-healing supramolecular polymers, Potential biomedical applications. (10 Lectures)

## **CHEMISTRY-DSE: BIOPHYSICAL CHEMISTRY (DSE2)**

**(Credits: Theory-05, Tutorials-01)**

**Theory -75 Lectures, Tutorial-15 h**

### **Conformation of proteins**

**(17 L)**

Ramachandran plot, secondary, tertiary and quarternary structure; domains; motif and folds. Thermodynamics of protein hydration.

### **Enzymes**

**(18 L)**

Introduction - chemical nature and general characterization - nomenclature, IUB system of enzyme classification, specificity, enzyme units, active site, mode of action - Lock and key theory and induced fit theory.



**Enzyme Kinetics** - Introduction to chemical kinetics, rate and order of reactions, factors affecting the enzyme activity, derivation of Michaelis - Menton Equation. Line - Weaver and Burk plot, Eadie- Hofstee plot. Enzyme inhibition - Competitive, non- competitive and uncompetitive inhibitions (kinetic derivations not required).

### **Membrane structure and functions**

**(20 L)**

Structure of model membrane, lipid bilayer and membrane protein diffusion, osmosis, ion channels, active transport, ion pumps, mechanism of sorting and regulation of intra-cellular transport, electrical properties of membranes.

### **Cell Signaling**

**(20 L)**

Hormones and their receptors, cell surface receptor, signaling through G-protein coupled receptors, signal transduction pathways, second messengers, regulation of signaling pathways, bacterial and plant two-component signaling systems, bacterial chemotaxis and quorum sensing.

### **Reference Book :**

- Charles R. Cantor , Paul R. Schimmel, Biophysical Chemistry (Part I,II,III), 11 th ed,W.H .Freeman and Company.
- D L Nelson, Cox Lehninger , Lehninger's Principles of Biochemistry ,4th ed , W H Freeman 2004.
- Jeremy M.Bug, John L.Tymoczko, Lubert Strye, Biochemistry, 5<sup>th</sup> ed, W.H .Freeman and Company.
- K.L.Kapoor,A Textbook of Physical Chemistry (Vol-5), Macmillan Publishers (India) Ltd.

## **CHEMISTRY-DSE: APPLICATIONS OF COMPUTERS IN CHEMISTRY(DSE3)**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

### **Basics:**

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

### **Numerical methods:**

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

*Differential calculus:* Numerical differentiation.

*Integral calculus:* Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

*Simultaneous equations:* Matrix manipulation: addition, multiplication. Gauss-Siedal method.

*Interpolation, extrapolation and curve fitting:* Handling of experimental data.

*Conceptual background of molecular modelling:* Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

### Reference Books:

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

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## PRACTICAL-DSE LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY

### 60 Lectures

Computer programs based on numerical methods for

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

### Reference Books:

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

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## CHEMISTRY-DSE: ANALYTICAL METHODS IN CHEMISTRY(DSE4)

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

**Qualitative and quantitative aspects of analysis:**

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

**(5 Lectures)**

**Optical methods of analysis:**

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

*UV-Visible Spectrometry:* Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

*Basic principles of quantitative analysis:* estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.

*Infrared Spectrometry:* Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Structural illustration through interpretation of data, Effect and importance of isotope substitution.

*Flame Atomic Absorption and Emission Spectrometry:* Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

**(25 Lectures)**

**Thermal methods of analysis:**

Theory of thermogravimetry (TG), basic principle of instrumentation.

Techniques for quantitative estimation of Ca and Mg from their mixture.

**(5 Lectures)**

**Electroanalytical methods:**

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK<sub>a</sub> values.

**(10 Lectures)**

**Separation techniques:**

Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

**(15 Lectures)**

### Reference Books:

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

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## PRACTICALS- DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

**60 Lectures**

### I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper Chromatographic separation of  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ , and  $\text{Cr}^{3+}$ .

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

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

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

### II. Solvent Extractions:

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

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

3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.

5. Analysis of soil:

- (i) Determination of pH of soil.
- (ii) Total soluble salt
- (iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

- (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
- (ii) Separation of metal ions from their binary mixture.
- (iii) Separation of amino acids from organic acids by ion exchange chromatography.

### III Spectrophotometry

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

### Reference Books:

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

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**CHEMISTRY-DSE: MOLECULAR MODELLING & DRUG DESIGN (DSE5)**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

### Introduction to Molecular Modelling:

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

**(10 Lectures)**

### Force Fields:

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

(14 Lectures)

### **Energy Minimization and Computer Simulation:**

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

(12 Lectures)

### **Molecular Dynamics & Monte Carlo Simulation:**

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

(12 Lectures)

### **Structure Prediction and Drug Design:**

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery — Chemoinformatics — QSAR.

(12 Lectures)

### **Reference Books:**

- AR. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
- J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
- Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer – Anamaya Publishers, 2008.

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## **PRACTICAL- DSE LAB: MOLECULAR MODELLING & DRUG DESIGN**

**60 Lectures**

- Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane bonds and ethene, ethyne, benzene and pyridine bonds.
- (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2—butene.
- Visualize the electron density and electrostatic potential maps for LiH, HF, N<sub>2</sub>, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- (a) Compare the shapes of the molecules: 1-butanol, 2—butanol, 2—methyl-1-propanol, and 2—methyl—2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d)

- amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
  - viii. Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
  - ix. (a) Compare the optimized bond angles H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

*Note:* Software: ChemSketch, ArgusLab ([www.planaria-software.com](http://www.planaria-software.com)), TINKER 6.2 ([dasher.wustl.edu/ffe](http://dasher.wustl.edu/ffe)), WebLab Viewer, Hyperchem, or any similar software.

### Reference Books:

- AR. Leach, *Molecular Modelling Principles and Application*, Longman, 2001.
- J.M. Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
- Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer – Anamaya Publishers, 2008.

## CHEMISTRY-DSE: NOVEL INORGANIC SOLIDS (DSE6)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### Synthesis and modification of inorganic solids:

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

(10 Lectures)

### Inorganic solids of technological importance:

Solid electrolytes — Cationic, anionic, mixed Inorganic pigments — coloured solids, white and black pigments. Molecular material and fullerenes, molecular materials & chemistry — one-dimensional metals, molecular magnets, inorganic liquid crystals.

(10 Lectures)

### Nanomaterials:

Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and antisil nanomaterials, bionano composites.

(10 Lectures)

### Introduction to engineering materials for mechanical construction:

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

(10 Lectures)

**Composite materials:**

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

(10 Lectures)

**Speciality polymers:**

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

(10 Lectures)

**Reference Books:**

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

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**CHEMISTRY PRACTICAL - DSE LAB: NOVEL INORGANIC SOLIDS****60 Lectures**

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

**Reference Book:**

- Fahlman, B.D. *Materials Chemistry*, Springer, 2004.

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**CHEMISTRY-DSE: POLYMER CHEMISTRY (CHDSE7)**

(Credits: Theory-06, Practicals-02)

Theory: 60 Lectures

**Introduction and history of polymeric materials:**

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

(4 Lectures)

**Functionality and its importance:**



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.

**(8 Lectures)**

**Kinetics of Polymerization:**

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.

**(8 lectures)**

**Crystallization and crystallinity:**

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

**(4 Lectures)**

Nature and structure of polymers-Structure Property relationships.

**(2 Lectures)**

**Determination of molecular weight of polymers** ( $M_n$ ,  $M_w$ , etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index.

**(8 Lectures)**

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

**(8 Lectures)**

**Polymer Solution** — 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.

**(8 Lectures)**

**Properties of Polymers** (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 polypyrrole, polythiophene)].

**(10 Lectures)**

## Reference Books:

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

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## CHEMISTRY PRACTICAL - DSE LAB: POLYMER CHEMISTRY

### 60 Lectures

#### 1. Polymer synthesis

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

#### Polymer characterization

1. Determination of molecular weight by viscometry:
  - (a) Polyacrylamide-anaNO<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

\*at least 7 experiments to be carried out.

### Reference Books:

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

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## CHEMISTRY-DSE: RESEARCH METHODOLOGY FOR CHEMISTRY(DSE8) (Credits: Theory-05, Tutorials-01)

### Theory: 75 Lectures

#### Literature Survey:

**Print:** Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

**Digital:** Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H—index, E—consortium, UGC infonet, E—books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki— Databases, ChemSpider, Science Direct, SciFinder, Scopus.

**Information Technology and Library Resources:** The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

(20 Lectures)

#### Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers — justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

(20 Lectures)

### **Chemical Safety and Ethical Handling of Chemicals:**

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric — safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

**(12 Lectures)**

### **Data Analysis**

*The Investigative Approach:* Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

*Analysis and Presentation of Data:* Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit,  $r$  and its abuse. Basic aspects of multiple linear regression analysis.

**(13 Lectures)**

### **Electronics**

Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

**(10 Lectures)**

### **Reference Books**

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2<sup>nd</sup> Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters — IUPAC — IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

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## **CHEMISTRY-DSE: GREEN CHEMISTRY(DSE9)**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

### **Introduction to Green Chemistry**

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

## (4 Lectures)

### Principles of Green Chemistry and Designing a Chemical synthesis

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

- 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.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity.  $\text{risk} = (\text{function}) \text{hazard} \times \text{exposure}$ ; waste or pollution prevention hierarchy.
- Green solvents— supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
- Energy requirements for reactions — alternative sources of energy: use of microwaves and ultrasonic energy.
- Selection of starting materials; avoidance of unnecessary derivatization — careful use of blocking/protecting groups.
- 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.
- 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.
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

## (30 Lectures)

### Examples of Green Synthesis/ Reactions and some real world cases

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 CO<sub>2</sub> 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

**(16 Lectures)**

### **Future Trends in Green Chemistry**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co crystal controlled solid state synthesis ( $C^2S^3$ ); Green chemistry in sustainable development.

**(10 Lectures)**

### **Reference Books:**

- Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
- Anastas, P.T. & Warner, J.K.: Green Chemistry - Theory and Practical, Oxford University Press (1998).
- Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
- Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
- Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2mi Edition, 2010.

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## **CHEMISTRY PRACTICAL - DSE LAB: GREEN CHEMISTRY**

**60 Lectures**

### **1. Safer starting materials**

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

### **2. Using renewable resources**

- Preparation of biodiesel from vegetable/ waste cooking oil.

### **3. Avoiding waste**

Principle of atom economy.

- Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.
- Preparation of propene by two methods can be studied
  - (I) Triethylamine ion +  $OH^-$  → propene + trimethylpropene + water
  - (II) 1-propanol  $\xrightarrow{H_2SO_4/\Delta}$  propene + water
- Other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

### **4. Use of enzymes as catalysts**

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

### **5. 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

## 6. Alternative sources of energy

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

## Reference Books:

- Anastas, P.T. & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
- Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. *Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi*. Bangalore CISBN 978-93-81141-55-7 (2013).
- Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2<sup>nd</sup> Edition, 2010.
- Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. *Introduction to Organic Laboratory Techniques: A Illicroscale and Macro Scale Approach*, W.B.Saunders, 1995.

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## CHEMISTRY-DSE: INDUSTRIAL CHEMICALS AND ENVIRONMENT(DSE10)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### Industrial Gases and Inorganic Chemicals

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

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

(10 Lectures)

### Industrial Metallurgy

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

(4 Lectures)

### Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

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

Pollution by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases. Methods of estimation of CO, NO<sub>x</sub>, SO<sub>x</sub> and control procedures.

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

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

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

Sludge disposal.

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

**(30 Lectures)**

### **Energy & Environment**

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

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

**(10 Lectures)**

### **Biocatalysis**

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

**(6 Lectures)**

### **Reference Books:**

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

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**CHEMISTRY PRACTICAL - DSE LAB: INDUSTRIAL CHEMICALS &**



## ENVIRONMENT

### 60 Lectures

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method ( $\text{AgNO}_3$  and potassium chromate).
6. Estimation of total alkalinity of water samples ( $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ) using double titration method.
7. Measurement of dissolved  $\text{CO}_2$ .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

### Reference Books:

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

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## CHEMISTRY-DSE: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE(DSE11)

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

### Silicate Industries

*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.

(16 Lectures)

### Fertilizers:

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.

**(8 Lectures)**

**Surface Coatings:**

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.

**(10 Lectures)**

**Batteries:**

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.

**(6 Lectures)**

**Alloys:**

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

**(10 Lectures)**

**Catalysis:**

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.

**(6 Lectures)**

**Chemical explosives:**

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

**(4 Lectures)**

**Reference Books:**

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Harwood Ltd. UK.
- R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
- J. A. Kent: *Riegel's Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New

Delhi.

- Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

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**PRACTICALS-DSE LAB: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

**60 Lectures**

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

**Reference Books:**

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

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**CHEMISTRY-DSE: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS(DSE12)**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

**Introduction to spectroscopic methods of analysis:**

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

**(4 Lectures)**

**Molecular spectroscopy:**

*Infrared spectroscopy:*

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection),

interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

*UV-Visible/ Near IR* — emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

**(16 Lectures)**

## **Separation techniques**

*Chromatography*: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.

### *Immunoassays and DNA techniques*

*Mass spectroscopy*: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

**(16 Lectures)**

Elemental analysis:

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

**(8 Lectures)**

**NMR spectroscopy**: Principle, Instrumentation, Factors affecting chemical shift, Spin- coupling, Applications.

**(4 Lectures)**

**Electroanalytical Methods**: Potentiometry & Voltammetry

**(4 Lectures)**

**Radiochemical Methods**

**(4 Lectures)**

**X-ray analysis and electron spectroscopy (surface analysis)**

**(4 Lectures)**

### Reference books:

- DA. Skoog, F.J. Holler & S. Crouch (ISBN 0-495-01201-7) *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.
- Willard, Merritt, Dean, Settle, *Instrumental Methods of Analysis*, 7<sup>th</sup> ed, IBH Book House, New Delhi.
- Atkins, P.W & Paula, J.D. *Physical Chemistry*, 10<sup>th</sup> Ed., Oxford University Press (2014).
- Kakkar, R. *Atomic and Molecular Spectroscopy: Concepts and Applications*. Cambridge University Press, 2015.
- Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed., Narosa (2004).
- Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4<sup>th</sup> Ed. Tata McGraw— Hill: New Delhi (2006).
- Smith, B.C. *Infrared Spectral Interpretations: A Systematic Approach*. CRC Press, 1998.
- Moore, W.J., *Physical Chemistry* Orient Blackswan, 1999.

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## PRACTICALS-DSE LAB: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

### 60 Lectures

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

*At least 10 experiments to be performed.*

**Reference Books:**

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

**CHEMISTRY-DSE: CHEMISTRY OF INORGANIC SOLIDS (DSE13)**

**(Credits: Theory-05; Tutorial-01)**

**Theory: 75 Lectures Tutorial-15 h**

Basic structures of Inorganic Solids

(22 L)

Some Basic Crystal Geometries: Simple cube (sc), body centred cube (bcc), face centred cube (fcc), diamond cube (dc), close packing models: hexagonal close packing (hcp) (ABAB... type), cubic close packing (ccp) (ABCABC... type) Tetrahedral and octahedral holes, packing efficiency.

Structural inferences (Simple) from crystallochemical parameters; Structure of Ionic Crystals: AB-type (i.e NaCl, CsCl and ZnS), AB<sub>2</sub> type (CaF<sub>2</sub>, SiO<sub>2</sub> and TiO<sub>2</sub>), Ilmenite and perovskite (ABO<sub>3</sub>).

Crystal Defects (Qualitative idea): Thermodynamics aspect of defects, Stoichiometric and nonstoichiometric, point defects, Schottky and Frenkel.

Synthesis and modification of inorganic solids:

(5 L)

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method.

Inorganic solids of technological importance:

(15 L)

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments. Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

Composite materials:

(15 L)

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

Speciality polymers:

(18 L)

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

**CHEMISTRY-DSE: CHEMISTRY OF NANOMATERIALS(DSE14)**

**(Credits: Theory-05; Tutorial-01)**

Theory: 75 Lectures Tutorial-15 h

**Unit-I: Basic Concepts on Nanomaterials**

(20 L)

The scope and challenges of nanomaterials chemistry, the nanoscale and colloidal systems, fundamentals of surface and interfacial chemistry, chemical potential and surface curvature, Young-Laplace equation, Kelvin equation and Gibbs-Thompson relation, Wulff plot, surface energy and stabilization of nanoscale materials, electrostatic stabilization, interaction between two suspended particles (DLVO theory), steric stabilization.

**Unit-II: Synthesis and Fabrication of Nanomaterials**

(20 L)

Top down and bottom up techniques, zero-dimensional nanomaterials: nanoparticles, synthesis of metallic, semiconducting and oxide nanoparticles, effect of reducing agent and stabilizer on particle size, one-dimensional nanostructures: nanowire and nanorods, fundamentals of VLS and SLS growth, electrospinning, two-dimensional nanostructures: thin films, physical and chemical vapor deposition (PVD and CVD), Diamond films, sol-gel films, Langmuir-Blodgett film.

**Unit-III: Special Nanoparticles**

(15 L)

Synthesis and detailed bonding features of carbon fullerenes and nanotubes, micro and mesoporous materials, core-shell structures, metal-polymer structures, organic-inorganic hybrids, intercalation compounds, nanocomposites.

**Unit-IV: Characterization, Properties and Applications of Nanomaterials**

(20 L)

X-ray Diffraction (XRD), Scherrer's Formula, scanning and tunneling electron Microscopy (preliminary idea), comparison of electronic band structures of nanomaterials (qualitative), size dependent properties: Electrical, optical, catalytic and magnetic properties of nanomaterials; superparamagnetism, melting point and lattice constants, nanobots, nanocatalysis, catalysis by gold nanoparticles, biological applications of nanoparticles.