

VIDYASAGAR UNIVERSITY



Curriculum for 3-Year B Sc (General) in

Chemistry

Under Choice Based Credit System (CBCS)
w.e.f 2018-2019

VIDYASAGAR UNIVERSITY

B Sc (General) in Chemistry

[Choice Based Credit System]

| Year | Semester | Course Type | Course Code | Course Title | Credit | L-T-P | Marks | | | | |
|------|----------|-----------------------------|-------------|---|--------|-----------------|-------|----|-----------|------------|--------------|
| 1 | I | SEMESTER-I | | | | | | | CA | ESE | TOTAL |
| | | Core-1 (DSC-1A) | | Atomic structure, Bonding, General organic chemistry & Aliphatic Hydrocarbons - Lab | 6 | 4-0-4 | 15 | 60 | 75 | | |
| | | Core-2 (DSC-2A) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | | |
| | | Core-3 (DSC-3A) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | | |
| | | AECC-1 (Elective) | | English/MIL | 2 | 1-1-0 | 10 | 40 | 50 | | |
| | | Semester - I : Total | | | | 20 | | | | 275 | |
| | II | SEMESTER-II | | | | | | | | | |
| | | Core-4 (DSC-1B) | | Chemical Energetics, Equilibria & Functional Organic Chemistry - Lab | 6 | 4-0-4 | 15 | 60 | 75 | | |
| | | Core-5 (DSC-2B) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | | |
| | | Core-6 (DSC-3B) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | | |
| | | AECC-2 (Elective) | | Environmental Studies | 4 | | 20 | 80 | 100 | | |
| | | Semester - 2 : Total | | | | 22 | | | | 325 | |

| Year | Semester | Course Type | Course Code | Course Title | Credit | L-T-P | Marks | | | |
|------|----------|-----------------------------|-------------|---|--------|-----------------|-------|-----------|------------|--------------|
| 2 | III | SEMESTER-III | | | | | | CA | ESE | TOTAL |
| | | Core-7 (DSC-1C) | | Conductance, Electrochemistry & Functional Organic Chemistry - Lab | 6 | 4-0-4 | 15 | 60 | 75 | |
| | | Core-8 (DSC-2C) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | Core-9 (DSC-3C) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | SEC-1 | | TBD | 2 | 1-1-0/ 1-0-2 | 10 | 40 | 50 | |
| | | Semester - 3 : Total | | | | 20 | | | | 275 |
| | IV | SEMESTER-IV | | | | | | | | |
| | | Core-10 (DSC-1D) | | Coordination chemistry, State of Matter and Chemical Kinetics - Lab | 6 | 4-0-4 | 15 | 60 | 75 | |
| | | Core-11 (DSC-2D) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | Core-12 (DSC-3D) | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | SEC-2 | | TBD | 2 | 1-1-0/ 1-0-2 | 10 | 40 | 50 | |
| | | Semester - 4 : Total | | | | 20 | | | | 275 |

| Year | Semester | Course Type | Course Code | Course Title | Credit | L-T-P | Marks | | | |
|------|-------------------------------|-----------------------------|-------------|-------------------------|------------|-----------------|-------|-----------|-------------|--------------|
| 3 | V | SEMESTER-V | | | | | | CA | ESE | TOTAL |
| | | DSE-1A | | Discipline-1(Chemistry) | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | DSE-2A | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | DSE-3A | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | SEC-3 | | TBD | 2 | 1-1-0/ 1-0-2 | 10 | 40 | 50 | |
| | | Semester - 5 : Total | | | | 20 | | | | 275 |
| | VI | SEMESTER-VI | | | | | | | | |
| | | DSE-1B | | Discipline-1(Chemistry) | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | DSE-2B | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | DSE-3B | | Other Discipline/TBD | 6 | 4-0-4/ 5-1-0 | 15 | 60 | 75 | |
| | | SEC-4 | | TBD | 2 | 1-1-0/ 1-0-2 | 10 | 40 | 50 | |
| | | Semester - 6 : Total | | | | 20 | | | | 275 |
| | Total in all semester: | | | | 122 | | | | 1700 | |

CC = Core Course , **AECC** = Ability Enhancement Compulsory Course , **GE** = Generic Elective , **SEC** = Skill Enhancement Course , **DSE** = Discipline Specific Elective , **CA**= Continuous Assessment , **ESE**= End Semester Examination , **TBD**=To be decided , **CT** = Core Theory, **CP**=Core Practical , **L** = Lecture, **T** = Tutorial , **P** = Practical , **MIL** = Modern Indian Language , **ENVS** = Environmental Studies .

List of Core and Elective Courses

Core Courses (CC)

- DSC-1A:** Atomic Structure, Bonding, general organic chemistry & aliphatic hydrocarbons
DSC-1B: Chemical Energetics, Equilibria & Functional Organic Chemistry
DSC-1C: Solutions, Phase equilibrium, Conductance, Electrochemistry & Functional Organic Chemistry
DSC-1D: Coordination Chemistry, States of matter Chemical Kinetics

Discipline Specific Electives (DSE)

- DSE-1:** Analytical Methods in Chemistry
Or
DSE-1: Polymer Chemistry
Or
DSE-1: Instrumental Methods of Chemical Analysis
Or
DSE-1: Organometallics, Bioinorganic Chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy
DSE-2: Applications of Computers in Chemistry.
Or
DSE-2: Green Chemistry
Or
DSE-2: Industrial Chemicals and Environment
Or
DSE-2: Quantum Chemistry, Spectroscopy & Photochemistry
Or
DSE-2: Molecular Modelling & Drug design

Skill Enhancement Course (SEC)

- SEC-1:** Basic Analytical Chemistry
Or
SEC-1: Chemo informatics
SEC-2: Analytical Clinical Biochemistry
Or
SEC-2: Intellectual Property Rights (IPR)
SEC-3: Pharmaceutical Chemistry
Or
SEC-3: Chemistry of Cosmetics & Perfumes
SEC-4: Pesticide Chemistry
Or
SEC-4: Fuel Chemistry

Core Courses (CC)

DSC-1A(CC-1): Atomic Structure, Bonding, general organic chemistry & aliphatic hydrocarbons Credits 06

DSC1AT: Atomic Structure, Bonding, general organic chemistry & aliphatic hydrocarbons Credits 04

Course Contents:

Section A: Inorganic Chemistry-I

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 ψ and ψ^2 , Schrödinger 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.

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 or $s-s$, $s-p$ 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^+ . Comparison of VB and MO approaches.

Section B: Organic Chemistry-I

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 Hückel's rule.

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). Threo 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).

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. KMnO₄) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC₂ 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 KMnO₄, ozonolysis and oxidation with hot alk. KMnO₄.

Suggested Readings:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.
- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
- Eliel, E.L. *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2000.
- Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
- Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

DSC1AP: Atomic structure, Bonding, general organic chemistry & aliphatic hydrocarbons (Practical) **Credits 02**

Practical:

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)
 - (a) Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
 - (b) Identify and separate the sugars present in the given mixture by paper chromatography.

Suggested Readings:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

DSC-1B (CC-2): Chemical Energetics, Equilibria & Functional Organic Chemistry **Credits 06**

DSC1BT: Chemical Energetics, Equilibria & Functional Organic Chemistry **Credits 04**

Course Contents:

Section A: Physical Chemistry-I

Chemical Energetic

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 – Kirchoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

Chemical Equilibrium:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG° , Le Chatelier's principle. Relationships between K_p , K_c and K_x for reactions involving ideal gases.

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.

Section B: Organic Chemistry-2

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-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (S_N1 , S_N2 and S_Ni) 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: KNH_2/NH_3 (or $NaNH_2/NH_3$). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

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. $KMnO_4$, acidic dichromate, conc. 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, NaHSO₃, NH₂-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Ponndorf Verley reduction.

Suggested Readings:

- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
- Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
- Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

DSC1BP: Chemical Energetics, Equilibria & Functional Organic Chemistry (Practical) Credits 02

Section A: Physical Chemistry

Thermo chemistry:

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO₃, NH₄Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH .

Ionic equilibria:

pH measurements

- a) Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.
- b) Preparation of buffer solutions:
 - (i) Sodium acetate-acetic acid
 - (ii) Ammonium chloride-ammonium hydroxide Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.
2. Criteria of Purity: Determination of melting and boiling points.
3. Preparations: Mechanism of various reactions involved to be discussed. Recrystallisation, determination of melting point and calculation of quantitative yields to be done.
 - (a) Bromination of Phenol/Aniline
 - (b) Benzoylation of amines/phenols
 - (c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone

Suggested Readings:

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

DSC-1C(CC-3): Solutions, Phase equilibrium, Conductance, Electrochemistry & Functional Organic Chemistry **Credits 06**

DSC1CT: Solutions, Phase equilibrium, Conductance, Electrochemistry & Functional Organic Chemistry **Credits 04**

Course Contents:

Section A: Physical Chemistry-2

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. Nernst distribution law and its applications, solvent extraction.

Phase Equilibrium

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, FeCl₃-H₂O and Na-K only).

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 acidbase).

Electrochemistry

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG , ΔH and ΔS 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).

Section B: Organic Chemistry-3

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 inter-conversion. *Reactions:* Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

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 HNO₂, Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

Diazonium salts: *Preparation:* from aromatic amines. *Reactions:* conversion to benzene, phenol, dyes.

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 – COOH group, acetylation of –NH₂ group, complexation with Cu²⁺ ions, ninhydrin test. Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by degradation Edmann degradation (Nterminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & Cactivating groups and Merrifield solid-phase synthesis.

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 disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

Suggested Readings:

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
- Mahan, B.H. *University Chemistry*, 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry*, 5th Ed., Macmillan Publishing Co.: New York (1985).
- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry (Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7th Ed.*, W. H. Freeman.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.

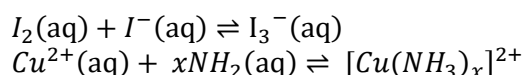
DSC-1CP: Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Organic Chemistry (Practical) Credits 02

Practical:

Section A: Physical Chemistry

Distribution

Study of the equilibrium of one of the following reactions by the distribution method:



Phase equilibria

- Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
- Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.
- Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Conductance

- Determination of cell constant
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
 - Strong acid vs. strong base
 - Weak acid vs. strong base

Potentiometry

Perform the following potentiometric titrations:

- Strong acid vs. strong base
- Weak acid vs. strong base
- Potassium dichromate vs. Mohr's salt

Section B: Organic Chemistry

I Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

II

- Separation of amino acids by paper chromatography
- Determination of the concentration of glycine solution by formylation method.
- Titration curve of glycine
- Action of salivary amylase on starch
- Effect of temperature on the action of salivary amylase on starch.
- Differentiation between a reducing and a nonreducing sugar.

Suggested Readings:

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

DSC-1D(CC-4):Coordination Chemistry, States of matter Chemical Kinetics
Credits 06

DSC1DT: Coordination Chemistry, States of matter Chemical Kinetics
Credits 04

Course Contents:

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).

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.

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 O_h and T_d complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

Section B: Physical Chemistry-3

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 CO₂. 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).

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).

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.

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).

Suggested Readings:

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley.
- Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
- Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd.
- Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008.

DSC1DP: Coordination Chemistry, States of matter & Chemical Kinetics (Practical)

Credits 02

Practical:

Section A: Inorganic Chemistry

Semi-micro qualitative analysis using H₂S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations : NH⁴⁺, Pb²⁺, Ag²⁺, Bi³⁺, Cu²⁺, Cd²⁺, Sn²⁺, Fe³⁺, Al³⁺, Co²⁺, Cr³⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺

Anions : CO₃²⁻, S²⁻, SO₃²⁻, S₂O₃²⁻, NO₃⁻, CH₃COO⁻, Cl⁻, Br⁻, I⁻, NO₂⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻

(Spot tests should be carried out wherever feasible)

1. Estimate the amount of nickel present in a given solution as bis (dimethylglyoximate) nickel(II) or aluminium as oximate in a given solution gravimetrically.
2. Draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound ($\text{KMnO}_4/\text{CuSO}_4$) and estimate the concentration of the same in a given solution.
3. Determine the composition of the Fe^{3+} -salicylic acid complex solution by Job's method.
4. Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
5. Estimation of total hardness of a given sample of water by complexometric titration.
6. Determination of concentration of Na^+ and K^+ using Flame Photometry.

Section B: Physical Chemistry

- (I) Surface tension measurement (use of organic solvents excluded).
- a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.
 - c) Study of the variation of surface tension of a detergent solution with concentration.
- (II) Viscosity measurement (use of organic solvents excluded).
- a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.
 - b) Study of the variation of viscosity of an aqueous solution with concentration of solute.
- (III) Chemical Kinetics

Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction
2. Integrated rate method:
 - a. Acid hydrolysis of methyl acetate with hydrochloric acid.
 - b. Saponification of ethyl acetate.
 - c. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate

Suggested Readings:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

Discipline Specific Electives (DSE)

DSE-1: Analytical Methods in Chemistry

Credits 06

DSE1T: Analytical Methods in Chemistry

Credits 04

Course Contents:

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.

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.

Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

Electro-analytical 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_a values.

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.

Suggested Readings:

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. *Vogel's Textbook of Quantitative Chemical Analysis*, John Wiley & Sons.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA,
- Christian, G.D; *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York.
- Harris, D. C. *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher.
- 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.
- Ditts, R.V. *Analytical Chemistry; Methods of Separation*, van Nostrand.

DSE1P: Analytical methods in Chemistry (Lab)

Credits 02

I. Separation Techniques

1. Chromatography:

- (a) Separation of mixtures
 - (i) Paper chromatographic separation of Fe^{3+} , Al^{3+} , and Cr^{3+} .
 - (ii) Separation and identification of the monosaccharide 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:

1. To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} -DMG complex in chloroform, and determine its concentration by spectrophotometry.
2. Solvent extraction of zirconium with amberliti LA-1, separation from a mixture of iron 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:
 1. Determination of pH of soil.
 2. Total soluble salt
 3. 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 pK_a 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.

Suggested Readings:

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. *Vogel's Textbook of Quantitative Chemical Analysis*, John Wiley & Sons.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA.
- Christian, Gary D; *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York.
- Harris, Daniel C: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman.
- Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age, International Publisher.
- 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.
- Ditts, R.V. *Analytical Chemistry; Methods of Separation*, van Nostrand.

Or

DSE-1: Polymer Chemistry

Credits 06

DSE1T: Polymer Chemistry

Credits 04

Course Contents:

Introduction and history of polymeric materials:

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

Functionality and its importance:

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

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.

Crystallization and crystallinity:

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

Nature and structure of polymers - Structure Property relationships.

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.

Glass transition temperature (T_g) and determination of T_g, Free volume theory, WLF equation, Factors affecting glass transition temperature (T_g).

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.

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)].

Suggested Readings:

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

DSE1P: Polymer Chemistry (Lab)

Credits 02

Practical:

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
3. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
 - a. Preparation of IPC
 - b. Purification of IPC
 - c. Interfacial polymerization
4. Redox polymerization of acrylamide
5. Precipitation polymerization of acrylonitrile
6. Preparation of urea-formaldehyde resin
7. Preparations of novalac resin/resold resin.
8. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:
 - (a) Polyacrylamide-aq. NaNO₂ 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.

Suggested Readings:

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

Or

DSE-1: Instrumental Methods of Chemical Analysis

Credits 06

DSE1T: Instrumental Methods of Chemical Analysis

Credits 04

Course Contents:

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.

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).

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).

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).

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

Electro analytical Methods: Potentiometry & Voltammetry

Radiochemical Methods.

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

Suggested Readings:

- 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*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- P.W. Atkins: *Physical Chemistry*.
- G.W. Castellan: *Physical Chemistry*.
- C.N. Banwell: *Fundamentals of Molecular Spectroscopy*.
- Brian Smith: *Infrared Spectral Interpretations: A Systematic Approach*.
- W.J. Moore: *Physical Chemistry*.

DSE1P: Instrumental Methods of Chemical Analysis (Lab)

Credits 02

Practical:

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 chromosomes)
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.

Suggested Readings:

- 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*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.

Or

DSE-1: Organometallics, Bioinorganic Chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy

Credits 06

DSE1T: Organometallics, Bioinorganic Chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy

Credits 04

Course Contents:

Section A: Inorganic Chemistry-4

Chemistry of 3d metals

Oxidation states displayed by Cr, Fe, Co, Ni and Co. A study of the following compounds (including preparation and important properties); Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, sodium nitroprusside $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$.

Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. AN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. p-acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies).

Bio-inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na^+ , K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Role of Ca^{2+} in blood clotting, stabilization of protein structures and structural role (bones).

Section B: Organic Chemistry - 4

Polynuclear and heteronuclear aromatic compounds:

Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism. *Reactions:* Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon).

Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions, λ_{\max} & ϵ_{\max} , chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λ_{\max} of conjugated dienes and α, β – unsaturated Compounds.

Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on $>C=O$ stretching absorptions).

Suggested Readings:

- James E. Huheey, Ellen Keiter & Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
- G.L. Miessler & Donald A. Tarr: *Inorganic Chemistry*, Pearson Publication.
- J.D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley & Sons.
- I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S.
- John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.
- R.M. Silverstein, G.C. Bassler & T.C. Morrill: *Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.
- R.T. Morrison & R.N. Boyd: *Organic Chemistry*, Prentice Hall.
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.

DSE-1P: Practical

Credits 02

Practical:

Section A: Inorganic Chemistry

1. Separation of mixtures by chromatography: Measure the R_f value in each case. (Combination of two ions to be given) Paper chromatographic separation of Fe^{3+} , Al^{3+} and Cr^{3+} or Paper chromatographic separation of Ni^{2+} , Co^{2+} , Mn^{2+} and Zn^{2+}
2. Preparation of any two of the following complexes and measurement of their conductivity:
 - (i) tetraamminecarbonatocobalt (III) nitrate
 - (ii) tetraamminecopper (II) sulphate
 - (iii) potassium trioxalatoferrate (III) trihydrate

Compare the conductance of the complexes with that of M/1000 solution of NaCl, $MgCl_2$ and

LiCl₃.

Section B: Organic Chemistry

Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

Suggested Readings:

- A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

DSE-2: Applications of computers in chemistry

Credits 06

DSE2T: Applications of computers in chemistry

Credits 04

Course Contents:

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 idea of molecular mechanics and practical MO methods.

Suggested Readings:

- Harris, D. C. *Quantitative Chemical Analysis*. 6th 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).

DSE1P: Applications of computers in chemistry (Lab)

Credits 02

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.

Suggested Readings:

- McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
- Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th 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).

Or

DSE-2: Green Chemistry

Credits 06

DSE2T: Green Chemistry

Credits 04

Course Contents:

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

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. Risk = (function) hazard × exposure; waste or pollution prevention hierarchy.

- Green solvents – supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solvent less 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 carbonyl) 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.

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 CO₂ for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azo pigments 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 interesterification for production of no Trans-Fats and Oils
9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

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 (C₂S₃); Green chemistry in sustainable development.

Suggested Readings:

- 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, 2nd Edition, 2010.

DSE2P: Green Chemistry (Lab)

Credits 02

Practical:

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 $\xrightarrow{\text{H}_2\text{SO}_4/\Delta}$ 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 CO₂ 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.

Suggested Readings:

- 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, 2nd Edition, 2010.
- Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. *Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach*, W.B.Saunders, 1995.

Or

DSE-2: Industrial Chemicals and Environment

Credits 06

DSE2T: Industrial Chemicals and Environment

Credits 04

Course Contents:

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.

Industrial Metallurgy

General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent. Hydrometallurgy, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond's process. Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

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 SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

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.

Biocatalysis

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

Suggested Readings:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood 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* 11th edition. Brooks/ Cole (2006).
- Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).

DSE2P: Industrial Chemicals & Environment

Credits 02

Practical:

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

Suggested Readings:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood 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.

Or

DSE-2: Quantum Chemistry, Spectroscopy & Photochemistry **Credits 06**

DSE2T: Quantum Chemistry, Spectroscopy & Photochemistry **Credits 04**

Course Contents:

Quantum Chemistry

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.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. 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.

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

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 wave functions, 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.

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.

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.

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, 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.

Suggested Readings:

- Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
- House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).
- Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
- Kakkar, R. *Atomic & Molecular Spectroscopy: Concepts & Applications*, Cambridge University Press (2015).

DSE2P: Practical

Credits 02

UV/Visible spectroscopy

- I. Study the 200-500 nm absorbance spectra of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1} , kJ mol^{-1} , cm^{-1} , eV).
- II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $\text{K}_2\text{Cr}_2\text{O}_7$.
- 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 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. Analyse the given vibration-rotation spectrum of HCl (g)

Suggested Readings:

- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).

Or

DSE-2: Molecular Modelling & Drug design

Credits 06

DSE2T: Molecular Modelling & Drug design

Credits 04

Course Contents:

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.

Force Fields:

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

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.

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.

Structure Prediction and Drug Design:

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

Suggested Readings:

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

DSE2P: Molecular Modelling & Drug design (Lab)

Credits 02

Practical:

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- ii. (a) Perform a conformational analysis of butane.
(b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character.
(b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule.
(b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound:
(a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene.
(b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se.
 (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), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Suggested Readings:

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

Skill Enhancement Course (SEC)

SEC-1: Basic Analytical Chemistry

Credits 02

SEC1T: Basic Analytical Chemistry

Credits 01

Course Contents:

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

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

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

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

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

Ion-exchange: Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics: Major and minor constituents and their function.

SEC1P: Practical

Credits 01

A:

1. Determination of pH of soil samples.

2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.
3. Determination of pH, acidity and alkalinity of a water sample.
4. Determination of dissolved oxygen (DO) of a water sample.
5. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
6. Analysis of preservatives and colouring matter.
7. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
8. To compare paint samples by TLC method.
9. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).
10. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
11. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

B:

Suggested Applications (Any one):

1. To study the use of phenolphthalein in trap cases.
2. To analyze arson accelerants.
3. To carry out analysis of gasoline.

C:

Suggested Instrumental demonstrations:

1. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.
2. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
3. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Suggested Readings:

- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*. 7th Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA.
- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth.
- Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
- Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
- Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
- Freifelder, D. *Physical Biochemistry 2nd Ed.*, W.H. Freeman and Co., N.Y. USA.
- Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA.
- Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall.
- Vogel, A. I. *Vogel's Quantitative Chemical Analysis 6th Ed.*, Prentice Hall.
- Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York.

Or

SEC-1: Chemo informatics

Credits 02

SEC1T: Chemo informatics

Course Contents:

Introduction to Chemo informatics:

History and evolution of chemo informatics, Use of chemo informatics, Prospects of chemo informatics, Molecular Modelling and Structure elucidation.

Representation of molecules and chemical reactions:

Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching chemical structures:

Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications:

Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

Suggested Readings:

- Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Chemoinformatics*. Springer: The Netherlands.
- Gasteiger, J. & Engel, T. (2003) *Chemoinformatics: A text-book*. Wiley-VCH.
- Gupta, S. P. (2011) *QSAR & Molecular Modeling*. Anamaya Pub.: New Delhi.

SEC-2: Intellectual Property Rights (IPR)

Credits 02

SEC2T: Intellectual Property Rights (IPR)

Course Contents:

Introduction to Intellectual Property: Historical Perspective, Different Types of IP, Importance of protecting IP.

Copyrights: Introduction, How to obtain, Differences from Patents.

Trade Marks: Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc. Differences from Designs.

Patents: Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Healthcare – balancing promoting innovation with public health, Software patents and their importance for India.

Geographical indications: Definition, rules for registration, prevention of illegal exploitation, importance to India.

Industrial Designs: Definition, How to obtain, features, International design registration.

Layout design of integrated circuits: Circuit Boards, Integrated Chips, Importance for electronic industry.

Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Different International agreements

(a) World Trade Organization (WTO):

- (i) General Agreement on Tariffs & Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement
- (ii) General Agreement on Trade related Services (GATS)
- (iii) Madrid Protocol
- (iv) Berne Convention
- (v) Budapest Treaty

(b) Paris Convention

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

IP Infringement issue and enforcement – Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property – Intangible assets and their valuation, Intellectual Property in the Indian Context – Various laws in India Licensing and technology transfer.

Suggested Readings:

- N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House .
- Manjula Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications.
- P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill.
- Arthur Raphael Miller, Micheal H.Davis; *Intellectual Property: Patents, Trademarks and Copyright in a Nutshell*, West Group Publishers (2000).
- Jayashree Watal, *Intellectual property rights in the WTO and developing countries*, Oxford University Press, Oxford.

Or

SEC-2: Analytical Clinical Biochemistry

Credits 02

SEC2T: Analytical Clinical Biochemistry

Credits 01

Course Contents:

Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins:

Review of concepts studied in the core course:

Carbohydrates: Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle. Isolation and characterization of polysachharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.

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

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying applications. Lipoproteins.

Hormone : Properties, functions and biochemical functions of steroid hormones. Biochemistry of peptide hormones.

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

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

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

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

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

SEC2P: Practical

Credit 01

Practical

Identification and estimation of the following:

1. Carbohydrates – qualitative and quantitative.

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

Suggested Readings:

- T.G. Cooper: Tool of Biochemistry.
- Keith Wilson and John Walker: Practical Biochemistry.
- Alan H Gowenlock: Varley's Practical Clinical Biochemistry.
- Thomas M. Devlin: Textbook of Biochemistry.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.
- Talwar, G.P. & Srivastava, M. *Textbook of Biochemistry and Human Biology*, 3rd Ed. PHI Learning.
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7th Ed.*, W. H. Freeman.
- Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.

SEC-3: Pharmaceutical Chemistry

Credits 02

SEC3T: Pharmaceutical Chemistry

Credits 01

Course Contents:

Drugs & Pharmaceuticals:

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, antiinflammatory agents (Aspirin, paracetamol, Ibuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation:

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

SEC3P: Practical

Credit 01

Practical:

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Suggested Readings:

- G.L. Patrick: Introduction to *Medicinal Chemistry*, Oxford University Press, UK.
- Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi.
- William O. Foye, Thomas L., Lemke, David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly Pvt. Ltd. New Delhi.

Or

SEC-3: Chemistry of Cosmetics & Perfumes

Credits 02

SEC3T: Chemistry of Cosmetics & Perfumes

Credits 01

Course Contents:

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmine, Civetone, Muscone.

SEC3P: Practical

Credit 01

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Suggested Readings:

- E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
- P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).

SEC-4: Pesticide Chemistry

Credits 02

SEC4T: Pesticide Chemistry

Credits 01

Course Contents:

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,);

Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

SEC4P: Practical

Credit 01

- 1 To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
- 2 Preparation of simple organophosphates, phosphonates and thiophosphates

Suggested Readings:

- Cremllyn, R. *Pesticides. Preparation and Modes of Action*, John Wiley & Sons, New York, 1978.

Or

SEC- 4: Fuel Chemistry

Credits 02

SEC4T: Fuel Chemistry

Course Contents:

Introduction: Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining. **Petroleum and Petrochemical Industry:** Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. **Petrochemicals:** Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene. **Lubricants:** Classification of lubricants, lubricating oils (conducting and non-conducting), Solid and semisolid lubricants, synthetic lubricants. Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Suggested Readings:

- Stocchi, E. *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK (1990).
- Jain, P.C. & Jain, M. *Engineering Chemistry* Dhanpat Rai & Sons, Delhi.
- Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut (1996).