

Proposed syllabus and Scheme of Examination

for

B.Sc. (Program) with Chemistry

Submitted

to

University Grants Commission

New Delhi

Under

Choice Based Credit System

April 2015

Details of Courses Under Undergraduate Program (B.Sc.)

Course	*Credits	
	Theory+ Practical	Theory+Tutorials
<u>I. Core Course</u>	12×4= 48	12×5=60
(12 Papers)		
04 Courses from each of the		
03 disciplines of choice		
Core Course Practical / Tutorial*	12×2=24	12×1=12
(12 Practical/ Tutorials*)		
04 Courses from each of the		
03 Disciplines of choice		
<u>II. Elective Course</u>	6×4=24	6×5=30
(6 Papers)		
Two papers from each discipline of choice		
including paper of interdisciplinary nature.		
Elective Course Practical / Tutorials*	6×2=12	6×1=6
(6 Practical / Tutorials*)		
Two Papers from each discipline of choice		
including paper of interdisciplinary nature		
<ul style="list-style-type: none"> • Optional Dissertation or project work in place of one Discipline elective paper (6 credits) in 6th Semester 		

III. Ability Enhancement Courses

1. Ability Enhancement Compulsory $2 \times 2 = 4$ $2 \times 2 = 4$

(2 Papers of 2 credits each)

Environmental Science

English/MIL Communication

2. Skill Enhancement Course $4 \times 2 = 8$ $4 \times 2 = 8$

(Skill Based)

(4 Papers of 2 credits each)

Total credit= 120

Total credit= 120

Institute should evolve a system/policy about ECA/ General Interest/Hobby/Sports/NCC/NSS/related courses on its own.

*wherever there is practical there will be no tutorials and vice -versa

Proposed scheme for choice based credit system in B. Sc. Program

	CORE COURSE (12)	Ability Enhancement Compulsory Course (AECC) (2)	Skill Enhancement Course (SEC) (2)	Discipline Specific Elective DSE (6)
I	DSC- 1 A Atomic Structure, Bonding, General Organic Chemistry & Aliphatic	(English/MIL Communication)/ Environmental Science		

	Hydrocarbons			
	DSC- 3 A			
II	DSC- 1 B	Environmental Science (English/MIL Communication)		
	Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I			
	DSC- 3 B			
III	DSC- 1 C		SEC-1	
	Solutions, Phase equilibrium, Conductance, Electrochemis- try & Functional Group Organic Chemistry-II			
	DSC- 3 C			
IV	DSC- 1 D		SEC -2	
	Chemistry of s- and p-block Elements, States of Matter & Chemical			

	Kinetics			
	DSC- 3 D			
V			SEC -3	DSE-1 A
				DSE-2 A
				DSE-3 A
VI			SEC -4	DSE-1 B
				DSE-2 B
				DSE-3 B

SEMESTER	COURSE OPTED	COURSE NAME	Credits
I	Ability Enhancement Compulsory Course-I	English/MIL communications/ Environmental Science	2
	Core Course-I	DSC 1A	6
	Core Course-II	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	4
	Core Course-II Practical/ Tutorial	Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons Lab	2
	Core Course-III	DSC 3A	6
II	Ability Enhancement Compulsory Course-II	English/MIL communications/ Environmental Science	2
	Core Course-IV	DSC 1B	6
	Core Course-V	Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I	4
	Core Course-V Practical/ Tutorial	Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I Lab	2
	Core Course-VI	DSC 3B	6
III	Core Course-VII	DSC 1C	6
	Core Course-VIII	Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry-II	4
	Core Course-VIII Practical/ Tutorial	Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry-II Lab.	2
	Core Course-IX	DSC 3C	6
	Skill Enhancement Course -1	SEC-1	2
IV	Core course-X	DSC 1D	6
	Core Course-XI	Chemistry of s- and p-block elements, States of matter & Chemical kinetics	4
	Course-XI Practical/Tutorial	Chemistry of s- and p-block elements, States of matter & Chemical kinetics Lab	2
	Core Course-XII	DSC 3D	6
	Skill Enhancement Course -2	SEC -2	2
V	Skill Enhancement Course -3	SEC -3	2
	Discipline Specific Elective -1	DSE-1A	6

	Discipline Specific Elective -2	DSE-2A	6
	Discipline Specific Elective -3	DSE-3A	6
VI	Skill Enhancement Course -4	SEC -4	2
	Discipline Specific Elective -4	DSE-1B	6
	Discipline Specific Elective -5	DSE-2B	6
	Discipline Specific Elective-6	DSE-3B	6
Total Credits			120

B.Sc. Program with Chemistry

Core papers Chemistry (Credit: 06 each) (CP 1-4):

1. Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons (4) + Lab (4)
2. Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I (4) + Lab (4)
3. Conductance, Electrochemistry & Functional Group Organic Chemistry-2 (4) + Lab (4)
4. Chemistry of s- and p-block elements, States of matter and Chemical Kinetics (4) + Lab (4)

Discipline Specific Elective papers (Credit: 06 each) (DSE 1, DSE 2): Choose 2

Chemistry

1. Applications of Computers in Chemistry (4) + Lab (4)
2. Analytical Methods in Chemistry (4) + Lab (4)
3. Molecular Modelling & Drug Design (4) + Lab (4)
4. Novel Inorganic Solids (4) + Lab (4)
5. Polymer Chemistry (4) + Lab (4)
6. Research Methodology for Chemistry (5) + Tutorials (1)
7. Green Chemistry (4) + Lab (4)
8. Industrial Chemicals & Environment (4) + Lab (4)
9. Inorganic Materials of Industrial Importance (4) + Lab (4)
10. Instrumental Methods of Analysis (4) + Lab (4)
11. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy (4) + Lab (4)
12. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy
13. Molecules of life (4) + Lab (4)
14. Dissertation

Note: Universities may include more options or delete some from this list

Skill Enhancement Course (any four) (Credit: 02 each)- SEC 1 to SEC 4

Chemistry

1. IT Skills for Chemists
2. Basic Analytical Chemistry
3. Chemical Technology & Society
4. Chemoinformatics
5. Business Skills for Chemists
6. Intellectual Property Rights
7. Analytical Clinical Biochemistry
8. Green Methods in Chemistry
9. Pharmaceutical Chemistry
10. Chemistry of Cosmetics & Perfumes
11. Pesticide Chemistry
12. Fuel Chemistry

Note: Universities may include more options or delete some from this list

Important:

1. **Each University/Institute should provide a brief write-up about each paper outlining the salient features, utility, learning objectives and prerequisites.**
2. **University can add/delete some experiments of similar nature in the Laboratory papers.**
3. **University can add to the list of reference books given at the end of each paper.**

Semester I

CHEMISTRY-DSC 2A: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Inorganic Chemistry-1 (30 Periods)

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

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of 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.

(14 Lectures)

Chemical Bonding and Molecular Structure

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

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

Concept of resonance and resonating structures in various inorganic and organic compounds.

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for *s-s*, *s-p* and *p-p* combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and NO⁺. Comparison of VB and MO approaches.

(16 Lectures)

Section B: Organic Chemistry-1 (30 Periods)

Fundamentals of Organic Chemistry

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

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

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

(8 Lectures)

Stereochemistry

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). 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).

(10 Lectures)

Aliphatic Hydrocarbons

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

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

Alkenes: (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO₄) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides.

Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO_4 , ozonolysis and oxidation with hot alk. KMnO_4 .

(12 Lectures)

Reference Books:

- J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
- F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
- T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
- I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
- R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

CHEMISTRY LAB: DSC 2A LAB: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

60 Lectures

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.

Reference Books:

- Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
- Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
- Textbook of Practical Organic Chemistry, A.I. Vogel, Prentice Hall, 5th edition.
- Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.

Semester II

CHEMISTRY-DSC 2B: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Physical Chemistry-I (30 Lectures)

Chemical Energetics

Review of thermodynamics and the Laws of Thermodynamics.

Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation.

Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

(10 Lectures)

Chemical Equilibrium:

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

(8 Lectures)

Ionic Equilibria:

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

(12 Lectures)

Section B: Organic Chemistry-2 (30 Lectures)

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

Aromatic hydrocarbons

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

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

(8 Lectures)

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (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.

(8 Lectures)

Alcohols, Phenols and Ethers (Upto 5 Carbons)

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

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO₄, acidic dichromate, conc. HNO₃). 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.

(14 Lectures)

Reference Books:

- T. W. Graham Solomons: *Organic Chemistry, John Wiley and Sons.*
- Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
- I.L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
- R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
- Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.
- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
- G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
- J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
- R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

CHEMISTRY LAB- DSC 2B LAB: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY

60 Lectures

Section A: Physical Chemistry

Thermochemistry

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 (KNO_3 , NH_4Cl).
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

Reference Books

- A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
- F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Semester III

CHEMISTRY-DSC 2C: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Physical Chemistry-2 (30 Lectures)

Solutions

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes.

Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. 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, $\text{FeCl}_3\text{-H}_2\text{O}$ 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 acid-base).

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 (30 Lectures)

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

Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic)

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Vohlard - Zelinsky Reaction.

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

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion.

Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

(6 Lectures)

Amines and Diazonium Salts

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

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction.

Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2 , Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

Diazonium salts: *Preparation:* from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

(6 Lectures)

Amino Acids, Peptides and Proteins:

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

Reactions of Amino acids: ester of -COOH group, acetylation of -NH_2 group, complexation with Cu^{2+} ions, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins.

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

(10 Lectures)

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

(8 Lectures)

Reference Books:

- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
 - G. W. Castellan: *Physical Chemistry* 4th Ed. Narosa (2004).
 - J. C. Kotz, P. M. Treichel, J. R. Townsend, *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
 - B. H. Mahan: *University Chemistry*, 3rd Edn. Narosa (1998).
 - R. H. Petrucci, *General Chemistry*, 5th Edn., 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* 7th Ed., W. H. Freeman
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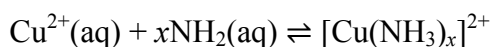
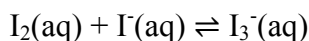
CHEMISTRY LAB-DSC 2C LAB: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & BIOMOLECULES

60 Lectures

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/nonreducing sugar.

Reference Books:

- A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman, 1960.

- B.D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
- Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.

Semester IV

CHEMISTRY-DSC 2D: CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon 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.

(4 Lectures)

s- and p-Block Elements

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochow scales). Allotropy in C, S, and P.

Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

Compounds of s- and p-Block Elements

Hydrides and their classification (ionic, covalent and interstitial), structure and properties with respect to stability of hydrides of p- block elements.

Concept of multicentre bonding (diborane).

Structure, bonding and their important properties like oxidation/reduction, acidic/basic nature of the following compounds and their applications in industrial, organic and environmental chemistry.

Hydrides of nitrogen (NH₃, N₂H₄, N₃H, NH₂OH)

Oxoacids of P, S and Cl.

Halides and oxohalides: PCl_3 , PCl_5 , SOCl_2 and SO_2Cl_2

(26 Lectures)

Section B: Physical Chemistry-3 (30 Lectures)

Kinetic Theory of Gases

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO_2 .

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).

Reference Books:

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

CHEMISTRY LAB-DSC 2D LAB: CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS

60 Lectures

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⁺, Ag⁺, 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⁻, NO₃⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, C₂O₄²⁻, F⁻

(Spot tests should be carried out wherever feasible)

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.
- b) 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 H₂SO₄ by studying kinetics of hydrolysis of methyl acetate

Reference Books:

- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Discipline Specific Elective

Select two papers

CHEMISTRY-DSE I-IV (ELECTIVES)

CHEMISTRY-DSE: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Basics:

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

Numerical methods:

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

Differential calculus: Numerical differentiation.

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

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

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

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

Reference Books:

- Harris, D. C. *Quantitative Chemical Analysis*. 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).
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PRACTICAL-DSE LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY

60 Lectures

Computer programs based on numerical methods for

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

Reference Books:

- McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
 - Mortimer, R. *Mathematics for Physical Chemistry*. 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).
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CHEMISTRY-DSE: ANALYTICAL METHODS IN CHEMISTRY (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Qualitative and quantitative aspects of analysis:

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

(5 Lectures)

Optical methods of analysis:

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

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

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

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

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

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

(25 Lectures)

Thermal methods of analysis:

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

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

(5 Lectures)

Electroanalytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

(10 Lectures)

Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique.

Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

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

Role of computers in instrumental methods of analysis.

(15 Lectures)

Reference Books:

- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- Ditts, R.V. Analytical Chemistry – Methods of separation.

PRACTICALS- DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

60 Lectures

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

- (i) Paper chromatographic separation of Fe^{3+} , Al^{3+} , and Cr^{3+} .
- (ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.
- (b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.
- (c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

- (i) To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} - DMG complex in chloroform, and determine its concentration by spectrophotometry.
 - (ii) Solvent extraction of zirconium with amberlite LA-1, separation from a mixture of irons and gallium.
3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.
4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.
5. Analysis of soil:
- (i) Determination of pH of soil.
 - (ii) Total soluble salt
 - (iii) Estimation of calcium, magnesium, phosphate, nitrate
6. Ion exchange:
- (i) Determination of exchange capacity of cation exchange resins and anion exchange resins.
 - (ii) Separation of metal ions from their binary mixture.
 - (iii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry

1. Determination of 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.

Reference Books:

- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- Ditts, R.V. Analytical Chemistry – Methods of separation.

**CHEMISTRY-DSE: MOLECULAR MODELLING & DRUG DESIGN
(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Introduction to Molecular Modelling:

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

(10 Lectures)

Force Fields:

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

(14 Lectures)

Energy Minimization and Computer Simulation:

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

(12 Lectures)

Molecular Dynamics & Monte Carlo Simulation:

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

(12 Lectures)

Structure Prediction and Drug Design:

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

Drug Discovery – Chemoinformatics – QSAR.

(12 Lectures)

Reference Books:

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

PRACTICAL- DSE LAB: MOLECULA MODELLING & DRUG DESIGN

60 Lectures

- Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b)

- Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- 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.

Reference Books:

- A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
 - J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
 - Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
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CHEMISTRY-DSE: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Synthesis and modification of inorganic solids:

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

(10 Lectures)

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerenes, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

(10 Lectures)

Nanomaterials:

Overview of nanostructures and nanomaterials: classification.

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

(10 Lectures)

Introduction to engineering materials for mechanical construction:

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

(10 Lectures)

Composite materials:

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

(10 Lectures)

Speciality polymers:

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

(10 Lectures)

Reference Books:

- Shriver & Atkins. Inorganic Chemistry, Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
- Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry.
- Frank J. Owens, Introduction to Nanotechnology

CHEMISTRY PRACTICAL - DSE LAB: NOVEL INORGANIC SOLIDS

60 Lectures

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

Reference Book:

- Fahan, *Materials Chemistry*, Springer (2004).
-

CHEMISTRY-DSE: POLYMER CHEMISTRY

(Credits: Theory-06, Practicals-02)

Theory: 60 Lectures

Introduction and history of polymeric materials:

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

(4 Lectures)

Functionality and its importance:

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

(8 Lectures)

Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

(8 lectures)

Crystallization and crystallinity:

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

(4 Lectures)

Nature and structure of polymers-Structure Property relationships.

(2 Lectures)

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

Polydispersity index.

(8 Lectures)

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

(8 Lectures)

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

(8 Lectures)

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties).

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes,

Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

(10 Lectures)

Reference Books:

- *Seymour's Polymer Chemistry*, Marcel Dekker, Inc.
- G. Odian: Principles of Polymerization, John Wiley.
- F.W. Billmeyer: Text Book of Polymer Science, John Wiley.
- P. Ghosh: Polymer Science & Technology, Tata Mcgraw-Hill.
- R.W. Lenz: Organic Chemistry of Synthetic High Polymers.

CHEMISTRY PRACTICAL - DSE LAB: POLYMER CHEMISTRY

60 Lectures

1. Polymer synthesis

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

Polymer characterization

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

Reference Books:

- Malcom P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)

- Petr Munk and Tejraj 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)
- Malcolm 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).

CHEMISTRY-DSE: RESEARCH METHODOLOGY FOR CHEMISTRY

(Credits: Theory-05, Tutorials-01)

Theory: 75 Lectures

Literature Survey:

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

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

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

(20 Lectures)

Methods of Scientific Research and Writing Scientific Papers:

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

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

(20 Lectures)

Chemical Safety and Ethical Handling of Chemicals:

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

(12 Lectures)

Data Analysis

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

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

(13 Lectures)

Electronics

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

(10 Lectures)

Reference Books

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 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.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

CHEMISTRY-DSE: GREEN CHEMISTRY
(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Introduction to Green Chemistry

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

(4 Lectures)

Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; 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); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, 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; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

(24 Lectures)

Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural.

2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols).

Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation.

Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.

3. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.

4. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of “Clayon”, a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

(24 Lectures)

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.

(8 Lectures)

Reference Books:

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

CHEMISTRY PRACTICAL - DSE LAB: GREEN CHEMISTRY

60 Lectures

1. Safer starting materials

The Vitamin C clock reaction using Vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- Effect of concentration on clock reaction
- Effect of temperature on clock reaction. (if possible)

2. Using renewable resources

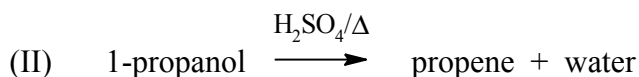
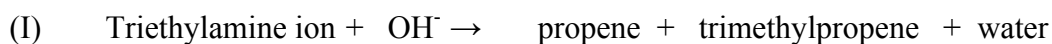
Preparation of biodiesel from vegetable oil.

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



The 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
Alternative Green solvents

5. Diels Alder reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

6. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
7. Mechanochemical solvent free synthesis of azomethines
8. Co-crystal controlled solid state synthesis (C²S³) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

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

Reference Books:

- Anastas, P.T. & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
- Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. *Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore* ISBN 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).
- Pavia, D. L. Lamponan, G. H. & Kriz, G.S. *W B Introduction to organic laboratory*

CHEMISTRY-DSE: INDUSTRIAL CHEMICALS AND ENVIRONMENT

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Industrial Gases and Inorganic Chemicals

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

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

(10 Lectures)

Industrial Metallurgy

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

(4 Lectures)

Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

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

Pollution by 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.

(30 Lectures)

Energy & Environment

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

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

(10 Lectures)

Biocatalysis

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

(6 Lectures)

Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis 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).
 - A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).
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CHEMISTRY PRACTICAL - DSE LAB: INDUSTRIAL CHEMICALS & ENVIRONMENT

60 Lectures

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

Reference Books:

- 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.
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CHEMISTRY-DSE: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

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

(16 Lectures)

Fertilizers:

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

(8 Lectures)

Surface Coatings:

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

(10 Lectures)

Batteries:

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

(6 Lectures)

Alloys:

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

(10 Lectures)

Catalysis:

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

Phase transfer catalysts, application of zeolites as catalysts.

(6 Lectures)

Chemical explosives:

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

(4 Lectures)

Reference Books:

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

60 Lectures

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

Reference Books:

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

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Introduction to spectroscopic methods of analysis:

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

(4 Lectures)

Molecular spectroscopy:

Infrared spectroscopy:

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

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

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

(16 Lectures)

Separation techniques

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

Immunoassays and DNA techniques

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

(16 Lectures)

Elemental analysis:

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence.

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

(8 Lectures)

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

(4 Lectures)

Electroanalytical Methods: Potentiometry & Voltammetry

(4 Lectures)

Radiochemical Methods

(4 Lectures)

X-ray analysis and electron spectroscopy (surface analysis)

(4 Lectures)

Reference books:

- Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
 - Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
 - 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.
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PRACTICALS-DSE LAB: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

60 Lectures

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

20. Laboratory analysis to confirm anthrax or cocaine
21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

At least 10 experiments to be performed.

Reference Books:

- Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

DSE: CHEMISTRY OF D-BLOCK ELEMENTS, QUANTUM CHEMISTRY & SPECTROSCOPY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Inorganic Chemistry-3 (30 Lectures)

Transition Elements (3d series)

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

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

(12 Lectures)

Coordination Chemistry

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

Drawbacks of VBT. IUPAC system of nomenclature.

(8 Lectures)

Crystal Field Theory

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for O_h and T_d complexes, Tetragonal distortion of octahedral geometry.

Jahn-Teller distortion, Square planar coordination.

(10 Lectures)

Section B: Physical Chemistry-4 (30 Lectures)

Quantum Chemistry & Spectroscopy

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. Born-Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.

Postulates of quantum mechanics, quantum mechanical operators.

Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, concept of zero-point energy.

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.

Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

(24 Lectures)

Photochemistry

Laws of photochemistry. Lambert-Beer's law. Fluorescence and phosphorescence. Quantum efficiency and reasons for high and low quantum yields. Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. Photoelectric cells.

(6 Lectures)

Reference Books:

- G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).
- G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).

- J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry*, Cengage Learning India Pvt. Ltd., New Delhi (2009).
- B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
- R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- J. D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Gary Wulfsberg: *Inorganic Chemistry*, Viva Books Pvt. Ltd.

DSE LAB

60 Lectures

Section A: Inorganic Chemistry

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

Section B: Physical Chemistry

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. Analyse the given vibration-rotation spectrum of HCl(g)

Reference Books:

- A.I. Vogel, Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.

- A.I. Vogel, Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

**DSE: ORGANOMETALLICS, BIOINORGANIC CHEMISTRY, POLYNUCLEAR HYDROCARBONS AND UV, IR SPECTROSCOPY
(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Section A: Inorganic Chemistry-4 (30 Lectures)

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, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$.

(6 Lectures)

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. EAN 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).

(12 Lectures)

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).

(12 Lectures)

Section B: Organic Chemistry-4 (30 Lectures)

Polynuclear and heteronuclear aromatic compounds:

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

(6 Lectures)

Active methylene compounds:

Preparation: Claisen ester condensation. Keto-enol tautomerism.

Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon).

(6 Lectures)

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).

(18 Lectures)

Reference Books:

- 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 LAB

60 Lectures

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 LiCl_3 .

Section B: Organic Chemistry

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

Reference Books:

- A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
- F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman (1960).

DSE: MOLECULES OF LIFE

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Carbohydrates

(10 Periods)

Classification of carbohydrates, reducing and non reducing sugars, General Properties of Glucose and Fructose, their open chain structure. Epimers, mutarotation and anomers. Determination of configuration of Glucose (Fischer proof).

Cyclic structure of glucose. Haworth projections. Cyclic structure of fructose.

Linkage between monosachharides, structure of disacharrides (sucrose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

Unit 2: Amino Acids, Peptides and Proteins

(12 Periods)

Classification of *Amino Acids*, Zwitterion structure and Isoelectric point.
Overview of Primary, Secondary, Tertiary and Quaternary structure of proteins.
Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C-terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis.

Unit 3: Enzymes and correlation with drug action (12 Periods)

Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action(Including stereospecificity) , Enzyme inhibitors and their importance, phenomenon of inhibition(Competitive and Non competitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of –OH group, –NH₂ group, double bond and aromatic ring,

Unit 4: Nucleic Acids (10 Periods)

Components of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), other components of nucleic acids, Nucleosides and nucleotides (**nomenclature**), Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA(**types of RNA**), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.

Unit 5: Lipids (8 Periods)

Introduction to lipids, classification.

Oils and fats: Common fatty acids present in oils and fats, Omega fatty acids, Trans fats, Hydrogenation, Saponification value, Iodine number.

Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol).

Unit 6: Concept of Energy in Biosystems (8 Periods)

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats.

Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change.

Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

Recommended Texts:

- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry (Volume I)*, 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 7th Ed.*, W. H. Freeman.

DSE LAB

60 Lectures

1. Separation of amino acids by paper chromatography
2. To determine the concentration of glycine solution by formylation method.
3. Study of titration curve of glycine
4. Action of salivary amylase on starch
5. Effect of temperature on the action of salivary amylase on starch.
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Differentiate between a reducing/ nonreducing sugar.
9. Extraction of DNA from onion/cauliflower
10. To synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Recommended Texts:

- Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
 - Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.
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Skill Enhancement Course (any four) (Credit: 02 each)- SEC1 to SEC4

Chemistry

IT SKILLS FOR CHEMISTS

(Credits: 02)

30 Lectures

Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms). Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary – bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Computer programming:

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.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

HANDS ON

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Handling numeric data: Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs. Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration-time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pK_a of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The t test. The F test.

Presentation: Presentation graphics

Reference Books:

- 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).

BASIC ANALYTICAL CHEMISTRY

(Credits: 02)

30 Lectures

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

- a. Determination of pH of soil samples.
- b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

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

- a. Determination of pH, acidity and alkalinity of a water sample.
- b. Determination of dissolved oxygen (DO) of a water sample.

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

- a. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- b. Analysis of preservatives and colouring matter.

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

- a. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
- b. To compare paint samples by TLC method.

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

- a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
- b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one):

- a. To study the use of phenolphthalein in trap cases.
- b. To analyze arson accelerants.
- c. To carry out analysis of gasoline.

Suggested Instrumental demonstrations:

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

- b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
- c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drink.

Reference Books:

1. Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.
 2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York.
 3. Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth (1992).
 4. Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
 5. Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
 6. Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
 7. Freifelder, D. *Physical Biochemistry 2nd Ed.*, W.H. Freeman and Co., N.Y. USA (1982).
 8. Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16 (1977).
 9. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall.
 10. Vogel, A. I. *Vogel's Quantitative Chemical Analysis 6th Ed.*, Prentice Hall.
 11. Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York (1995).
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CHEMICAL TECHNOLOGY & SOCIETY (Credits: 02)

Theory: 30 Lectures

Chemical Technology

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Society

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants); energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission; materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs.

Reference Book:

CHEMOINFORMATICS

(Credits: 02)

Theory: 30 Lectures

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, 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.

Hands-on Exercises

Reference Books:

- 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.
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BUSINESS SKILLS FOR CHEMISTS

(Credits: 02)

Theory: 30 Lectures

Business Basics

Key business concepts: Business plans, market need, project management and routes to market.

Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in India and global economies.

Making money

Financial aspects of business with case studies

Intellectual property

Concept of intellectual property, patents.

Reference

www.rsc.org

INTELLECTUAL PROPERTY RIGHTS (IPR) (Credits: 02)

Theory: 30 Lectures

In this era of liberalization and globalization, the perception about science and its practices has undergone dramatic change. The importance of protecting the scientific discoveries, with commercial potential or the intellectual property rights is being discussed at all levels – statutory, administrative, and judicial. With India ratifying the WTO agreement, it has become obligatory on its part to follow a minimum acceptable standard for protection and enforcement of intellectual property rights. The purpose of this course is to apprise the students about the multifaceted dimensions of this issue.

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.

Reference Books:

- N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).

- Manjula Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).
- P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill (2001).
- 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.

ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 02)

THEORY: 30 Lectures

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.

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. 6. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

Practicals

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

Reference Books:

- 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.
- Jeremy M. Berg, John L Tymoczko, Lubert Stryer: Biochemistry.
- G. P. Talwar and M Srivastava: Textbook of Biochemistry and Human Biology.
- A.L. Lehninger: Biochemistry.
- O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.

GREEN METHODS IN CHEMISTRY

(Credits: 02)

Theory: 30 Lectures

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

The following Real world Cases in Green Chemistry should be discussed:

- 1 A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
- 2 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- 3 Environmentally safe antifoulant.
- 4 CO₂ as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.

- 5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
- 6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
- 7 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- 8 Development of a fully recyclable carpet: cradle to cradle carpeting.

Reference Books:

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press
2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New

PHARMACEUTICAL CHEMISTRY

(Credits: 02)

Theory: 30 Lectures

Drugs & Pharmaceuticals

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory 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.

Practicals

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

Reference Books:

- 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.

CHEMISTRY OF COSMETICS & PERFUMES

(Credits: 02)

30 Lectures

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, Jasmone, Civetone, Muscone.

Practicals

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.

Reference Books:

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

(Credits: 02)

30 Lectures

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).

Practicals

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

Reference Book:

- R. Cremlyn: *Pesticides*, John Wiley.
-

FUEL CHEMISTRY

(Credits: 02)

30 Lectures

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.

Reference Books:

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