

**Proposed syllabus and Scheme of Examination
for
B.Sc. (Honours) Chemistry**

Submitted to
University of Delhi
Delhi

Under
Choice Based Credit System

June 2015

CHOICE BASED CREDIT SYSTEM

B.Sc. HONOURS WITH CHEMISTRY

Course Structure (Chemistry-Major)

Details of courses under B.Sc. (Honours)

Course	Theory+ Practical	Credits
I. Core Course Theory (14 Papers)		$14 \times 4=56$
Core Course Practical (14 Papers)		$14 \times 2=28$
	Total:	84

II. Elective Course (8 Papers)

A. 1. Discipline Specific Elective (DSE) Theory (4 Papers)		$4 \times 4=16$
A. 2. Discipline Specific Elective (DSE) Practical (4 Papers)		$4 \times 2=8$
B. 1. Generic Elective (GE)/ Interdisciplinary Theory (4 Papers)		$4 \times 4=16$ $4 \times 5=20$
B. 2. Generic Elective (GE) Practical/Tutorial* (4 Papers)		$4 \times 2=8$ $4 \times 1=4$
	Total:	48

Optional Dissertation or project work in place of one Discipline Specific Elective Paper. (6 credits) in 6th Semester

III. Ability Enhancement Courses (4 Papers)

1. Ability Enhancement Compulsory (2 Papers of 2 credits each) Environmental Science English/MIL Communication		$2 \times 2=4$
2. Ability Enhancement Elective (Skill Based) (2 Papers of 2 credits each) (Minimum 2)		$2 \times 2=4$
	Total:	08

Total credit **140**

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

SEMESTER	COURSE OPTED	COURSE NAME	Credits
I	AEC-I Compulsory	English Communications/ Environmental Science	2
	Core Course-I	Inorganic Chemistry-I	4
	Core Course-I Practical	Inorganic Chemistry-I Lab	2
	Core Course-II	Physical Chemistry-I	4
	Core Course-II Practical	Physical Chemistry-I Lab	2
	Generic Elective -1 GE-1		4/5
	Generic Elective -1 Practical/Tutorial		2/1
II	AEC-II Compulsory	Environmental Science English Communications	2
	Core Course-III	Organic Chemistry-I	4
	Core Course-III Practical	Organic Chemistry-I Lab	2
	Core Course-IV	Physical Chemistry-II	4
	Core Course-IV Practical	Physical Chemistry-II Lab	2
	Generic Elective -2 GE-2		4/5
	Generic Elective -2 Practical/Tutorial		2/1
III	Core Course-V	Inorganic Chemistry-II	4
	Core Course-V Practical	Inorganic Chemistry-II Lab	2
	Core Course-VI	Organic Chemistry-II	4
	Core Course-VI Practical	Organic Chemistry-II Lab	2
	Core Course-VII	Physical Chemistry-III	4
	Core Course-VII Practical	Physical Chemistry-III Lab	2
	Skill Enhancement Course -1 SEC-1		2
Generic Elective -3	GE-3	4/5	
Generic Elective -3	Practical/Tutorial	2/1	
IV	Core Course-VIII	Inorganic Chemistry-III	4
	Course-VIII Practical	Inorganic Chemistry-III Lab	2
	Core Course-IX	Organic Chemistry-III	4
	Course-IX Practical	Organic Chemistry-III Lab	2
	Core Course-X	Physical Chemistry-IV	4
	Course-X Practical	Physical Chemistry-IV Lab	2

	Skill Enhancement Course -2 SEC -2	2
	Generic Elective -4 GE-4	4/5
	Generic Elective -4 Practical	2/1
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V	Core Course-XI Organic Chemistry-IV	4
	Core Course-XI Practical Organic Chemistry-IV Lab	2
	Core Course-XII Physical Chemistry-V	4
	Core Course-XII Practical Physical Chemistry-V Lab	2
	Discipline Specific Elective -1 DSE-1	4
	Discipline Specific Elective -1	
	Practical/Tutorial DSE-1 Lab	2
	Discipline Specific Elective -2 DSE-2	4
	Discipline Specific Elective- 2	
	Practical/Tutorial DSE-2 Lab	2
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VI	Core Course-XIII Inorganic Chemistry-IV	4
	Core Course-XIII Practical Inorganic Chemistry-IV Lab	2
	Core Course-XIV Organic Chemistry-V	4
	Core Course-XIV Practical Organic Chemistry-V Lab	2
	Discipline Specific Elective -3 DSE-3	4
	Discipline Specific Elective -3	
	Practical/Tutorial DSE-3 Lab	2
	Discipline Specific Elective-4 DSE-4	4
	Discipline Specific Elective -4	
	Practical/Tutorial DSE-4 Lab	2
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	Total Credits	140

Core Papers (C): (Credit: 06 each)

(4 Lectures/week for Theory and 4 Periods/week for practical)

1. Inorganic Chemistry I: Atomic Structure & Chemical Bonding (4 + 4)
2. Physical Chemistry I: States of Matter & Ionic Equilibrium (4 + 4)
3. Organic Chemistry I: Basics and Hydrocarbons (4 + 4)
4. Physical Chemistry II: Chemical Thermodynamics and its Applications (4 + 4)
5. Inorganic Chemistry II: s- and p-Block Elements (4 + 4)
6. Organic Chemistry II: Oxygen Containing Functional Groups (4 + 4)
7. Physical Chemistry III: Phase Equilibria and Electrochemical Cells (4 + 4)
8. Inorganic Chemistry III: Coordination Chemistry (4 + 4)

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| 9. Organic Chemistry III: | Heterocyclic Chemistry (4 + 4) |
| 10. Physical Chemistry IV: | Conductance & Chemical Kinetics (4 + 4) |
| 11. Organic Chemistry IV: | Biomolecules (4 + 4) |
| 12. Physical Chemistry V: | Quantum Chemistry & Spectroscopy (4 + 4) |
| 13. Inorganic Chemistry IV: | Organometallic Chemistry (4 + 4) |
| 14. Organic Chemistry V: | Spectroscopy (4 + 4) |

**Discipline Specific Elective Papers: (Credit: 06 each) (4 papers to be selected)-
DSE 1-4**

DSE 1: Any one of the following

1. Novel Inorganic Solids (4) + Lab (4)
2. Inorganic Materials of Industrial Importance (4) + Lab (4)

DSE 2-4: Choose any three of the following

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. Polymer Chemistry (4) + Lab (4)
5. Research Methodology for Chemistry (5) + Tutorials (1)
6. Green Chemistry (4) + Lab (4)
7. Industrial Chemicals & Environment (4) + Lab (4)
8. Instrumental Methods of Analysis (4) + Lab (4)
9. Dissertation

Other Discipline (Four papers of any one discipline)- GE 1 to GE 4

1. Mathematics (5) + Tut (1)
2. Physics (4) + Lab (4)
3. Economics (5) + Tut (1)
4. Computer Science (4) + Lab (4)

**Skill Enhancement Courses (02 to 04 papers) (Credit: 02 each)- SEC1 to SEC4
(Emphasis should be given to Hands on Exercises) (Hands on except for papers
3, 5 and 6)**

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

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

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. Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II (4) + Lab (4)
4. Chemistry of s- and p-block elements, States of matter and Chemical Kinetics (4) + Lab (4).
5. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy (4) + Lab (4)
6. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy (4) + Lab (4)
7. Molecules of life (4) + Lab (4).

At least two mathematics papers are compulsory for admission for MSc Chemistry in Delhi University.

Discipline (Two Mathematics papers compulsory, two papers of one other discipline may be selected)- GE 1 to GE

CORE COURSE (HONOURS IN CHEMISTRY)

SEMESTER I

CHEMISTRY - C I: *INORGANIC CHEMISTRY-I* (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Atomic Structure: *Recapitulation of Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance.*

Schrödinger's wave equation, significance of ψ and ψ^2 . Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, aufbau principle and its limitations.

(14 Lectures)

Periodicity of Elements: Brief discussion of the following properties of the elements, with reference to *s* & *p*-block and the trends shown:

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Atomic and ionic radii

(c) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization enthalpy and trends in groups and periods.

(d) Electron gain enthalpy and trends in groups and periods.

(e) Electronegativity, Pauling's/ Allred Rochow's scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity.

(16 Lectures)

Chemical Bonding:

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

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule,

Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2 , O_2 , C_2 , B_2 , F_2 , CO , NO , and their ions; HCl (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of the following simple molecules and ions containing lone pairs and bond pairs of electrons: H_2O , NH_3 , PCl_3 , PCl_5 , SF_6 , ClF_3 , I_3^- , BrF_2^+ , PCl_6^- , ICl_2^- , ICl_4^- and SO_4^{2-} .

Multiple bonding (σ and π bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

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

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

(30 Lectures)

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry, Pearson Education 2010
- Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K. Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education 2006.
- Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Shriver, D.D. & P. Atkins, *Inorganic Chemistry 2nd Ed.*, Oxford University Press, 1994.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.

Practical C – I Lab: 60 Lectures

(A) Titrimetric Analysis

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

(B) Acid-Base Titrations

Principles of acid-base titrations to be discussed.

- (i) Estimation of sodium carbonate using standardized HCl .
- (ii) Estimation of carbonate and hydroxide present together in a mixture.
- (iii) Estimation of carbonate and bicarbonate present together in a mixture.
- (iv) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

Principles of oxidation-reduction titrations (electrode potentials) to be discussed.

- (i) Estimation of Fe(II) and oxalic acid using standardized KMnO_4 solution
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
- (iii) Estimation of Fe(II) with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator (diphenylamine, N-phenylanthranilic acid) and discussion of external indicator.

Reference Books:

- Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.
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CHEMISTRY - C II: *PHYSICAL CHEMISTRY I* **(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Gaseous state: Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η ; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z , and its variation with pressure and temperature for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour, calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states. **(18 Lectures)**

Liquid state: Qualitative treatment of the structure of the liquid state; physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. **(6 Lectures)**

Solid state: Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and

powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

(16 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; dissociation constants of mono and diprotic acids. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

(20 Lectures)

Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry Ed., Oxford University Press 13 (2006).
- Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).

Practical C – II Lab: 60 Lectures

1. Surface tension measurements using stalagmometer.

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

2. Viscosity measurement using Ostwald's viscometer.

- a. Determination of co-efficient of viscosity of an unknown aqueous solution.
- b. Study the variation of co-efficient of viscosity with different concentration of Poly Vinyl Alcohol (PVA) and determine molar of PVA.
- b. Study the variation of viscosity with different concentration of sugar solutions.

3. Solid State:

- a. Indexing of a given powder diffraction pattern of a cubic crystalline system.

4. pH metry:

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

b. Preparation of buffer solutions of different pH values i. Sodium acetate-acetic acid ii. Ammonium chloride-ammonium hydroxide

c. pH metric titration of (i) strong acid with strong base, (ii) weak acid with strong base. Determination of dissociation constant of a weak acid.

Any other experiment carried out in the class.

Reference Books:

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

SEMESTER II

CHEMISTRY - C III: *ORGANIC CHEMISTRY I* **(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Recapitulation of basics of Organic Chemistry

Hybridization, Shapes of molecules

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation Dipole moment; Hydrogen bonding (Applications to be discussed with relevant topics)

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

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

(6 Lectures)

Stereochemistry:

Fischer, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis-trans, syn-anti and E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and their resolution. Relative and absolute configuration: D/L and R/S designations.

(18 Lectures)

Chemistry of Aliphatic Hydrocarbons

A. Carbon-Carbon sigma bonds

General methods of preparation, physical and chemical properties of alkanes: Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation -relative reactivity and selectivity.

B. Carbon-Carbon pi bonds:

General methods of preparation, physical and chemical properties of alkenes and alkynes, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation(oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

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

C. Cycloalkanes and Conformational Analysis

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

(24 Lectures)

Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

(12 Lectures)

Reference Books:

- Morrison, R. N. & 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: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds; Wiley: London, 1994.
- Kalsi, P. S. Stereochemistry Conformation and Mechanism; New Age International, 2005.

Practical C – III Lab: 60 Lectures

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
 - a. Water
 - b. Alcohol
 - c. Alcohol-Water
3. Determination of the melting points of unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
4. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds
5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)
6. Chromatography
 - a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
 - b. Separation of a mixture of two sugars by ascending paper chromatography
 - c. Separation of a mixture of o- and p-nitrophenol or o- and p-aminophenol by thin layer chromatography (TLC)
7. Detection of extra elements
8. Organic Preparations
 - (i) Bromination of acetanilide / aniline / phenol
 - (ii) Nitration of nitrobenzene / toluene.

Reference Books

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
 - Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
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CHEMISTRY - C IV: PHYSICAL CHEMISTRY II (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Chemical Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems.

First law: Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, calculations of Q, W, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Thermochemistry: Heats of reactions: standard states; enthalpy of formation and enthalpy of combustion and its applications; effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions.

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

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules. Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

(36 Lectures)

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

(8 Lectures)

Chemical Equilibrium: Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration (Le Chatelier Principle, Quantitatively). Free energy of mixing and spontaneity. equilibrium between ideal gases and a pure condensed phase.

(8 Lectures)

Solutions and Colligative Properties: Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

(8 Lectures)

Reference Books:

- Peter, A. & Paula, J. de. Physical Chemistry 9th Ed., Oxford University Press (2011).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi (2004).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Levine, I. N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
- Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006)

Practical C – IV Lab: 60 Lectures

Thermochemistry:

- (a) Determination of heat capacity of a calorimeter for different volumes using (i) change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution of sulphuric acid or enthalpy of neutralization), and (ii) heat gained equal to heat lost by cold water and hot water respectively
- (b) Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- (c) Determination of the enthalpy of ionization of ethanoic acid.
- (d) Determination of integral enthalpy (endothermic and exothermic) solution of salts.
- (e) Determination of basicity of a diprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- (f) Determination of enthalpy of hydration of salt.
- (g) Study of the solubility of benzoic acid in water and determination of ΔH .

Any other experiment carried out in the class.

Reference Books:

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

CHEMISTRY - C V: *INORGANIC CHEMISTRY II* **(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 and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy with reference to cyanide process for silver and gold. Methods of purification of metals: Electrolytic process, van Arkel-de Boer process and Mond's process, Zone refining.

(6 Lectures)

Chemistry of s Block Elements:

- (i) General characteristics: melting point, flame colour, reducing nature, diagonal relationships and anomalous behavior of first member of each group.
- (ii) Reactions of alkali and alkaline earth metals with oxygen, hydrogen, nitrogen and water.
- (iii) Common features such as ease of formation, thermal stability and solubility of the following alkali and alkaline earth metal compounds: hydrides, oxides, peroxides, superoxides, carbonates, nitrates, sulphates.
- (iv) Complex formation tendency of s-block elements; structure of the following complexes: crown ethers and cryptates of Group I; basic beryllium acetate, beryllium nitrate, EDTA complexes of calcium and magnesium.
- (v) Solutions of alkali metals in liquid ammonia and their properties.

(22 Lectures)

Chemistry of p Block Elements:

Electronic configuration, atomic and ionic size, metallic/non-metallic character, melting point, ionization enthalpy, electron gain enthalpy, electronegativity, Allotropy of C, P, S; inert pair effect, diagonal relationship between B and Si and anomalous behaviour of first member of each group.

(6 lectures)

Structure, bonding and properties: acidic/basic nature, stability, ionic/covalent nature, oxidation/reduction, hydrolysis, action of heat of the following:

- Hydrides: hydrides of Group 13 (only diborane), Group 14, Group 15 (EH_3 where E = N, P, As, Sb, Bi), Group 16 and Group 17.
- Oxides: oxides of phosphorus, sulphur and chlorine
- Oxoacids: oxoacids of phosphorus and chlorine; peroxyacids of sulphur
- Halides: halides of silicon and phosphorus

Preparation, properties, structure and uses of the following compounds:

- Borazine
- Silicates, silicones,
- Phosphonitrilic halides $\{(\text{PNCl}_2)_n \text{ where } n = 3 \text{ and } 4\}$
- Interhalogen and pseudohalogen compounds
- Clathrate compounds of noble gases, xenon fluorides (MO treatment of XeF_2).

(26 Lectures)

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry, Pearson Education 2010
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry 3rd Ed.*, John Wiley Sons, N.Y. 1994.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth- Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 3rd Ed.(adapted)*, Pearson, 2009
- Shriver, D.F., Atkins P.W and Langford, C.H., *Inorganic Chemistry 2nd Ed.*, Oxford University Press, 1994

Practical C – V Lab: 60 Lectures

(A) Iodo / Iodimetric Titrations

- (i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodometrically).
- (ii) Estimation of antimony in tartar-emetic iodimetrically

(B) Complexometric titrations using disodium salt of EDTA

- (i) Estimation of Mg^{2+} , Zn^{2+}
- (ii) Estimation of Ca^{2+} by substitution method

(C) Inorganic preparations

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

Reference Books:

- Vogel, A.I. *A Textbook of Quantitative Inorganic Analysis*, ELBS. 1978
 - Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.
-

CHEMISTRY - C VI: ORGANIC CHEMISTRY II **(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Chemistry of Halogenated Hydrocarbons:

Alkyl halides: Methods of preparation and properties, nucleophilic substitution reactions – S_N1 , S_N2 and S_{Ni} mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; S_{NAr} , Benzyne mechanism.

Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Organometallic compounds of Mg (Grignard reagent) – Use in synthesis of organic compounds.

(16 Lectures)

Alcohols, Phenols, Ethers and Epoxides:

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

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

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and LiAlH_4

(16 Lectures)

Carbonyl Compounds:

Structure, reactivity, preparation and properties;

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α - substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, LiAlH_4 , NaBH_4 , MPV, PDC)

Addition reactions of α , β - unsaturated carbonyl compounds: Michael addition.

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

(16 Lectures)

Carboxylic Acids and their Derivatives:

General methods of preparation, physical properties and reactions of monocarboxylic acids, effect of substituents on acidic strength. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids.

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

(12 Lectures)

Reference Books:

- 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).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.

Practical C – VI Lab: 60 Lectures

1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.
2. Organic preparations:

- i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and phenols (β -naphthol, vanillin, salicylic acid) by any one method:
 - a. Using conventional method.
 - b. Using green approach
- ii. Benzoylation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction.
- iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
- iv. Selective reduction of meta dinitrobenzene to m-nitroaniline.
- v. Hydrolysis of amides and esters.
- vi. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
- vii. S-Benzylisothiuronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
- viii. Aldol condensation using either conventional or green method.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization and melting point.

Reference Books:

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

CHEMISTRY - C VII: PHYSICAL CHEMISTRY III (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Phase Equilibria: Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems (H_2O and S), with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points. Three component systems: triangular plots, water-chloroform-acetic acid system. Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible

liquids (ideal and non ideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation. Nernst distribution law: its derivation and applications. **(27 Lectures)**

Electrochemical Cells: Rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and $\text{SbO/Sb}_2\text{O}_3$ electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). **(27 Lectures)**

Surface chemistry: Physical adsorption, chemisorption, adsorption isotherms (Langmuir and Freundlich). nature of adsorbed state. Qualitative discussion of BET. **(6 Lectures)**

Reference Books:

- Peter Atkins & Julio De Paula, Physical Chemistry 9th Ed., Oxford University Press (2010).
- Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
- McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- Ball, D. W. Physical Chemistry Cengage India (2012).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
- Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

Practical C – VII Lab: 60 Lectures

Phase Equilibria:

- I. Determination of critical solution temperature and composition at CST of the phenol-water system and to study the effect of impurities of sodium chloride and succinic acid on it.
- II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method: a. simple eutectic and b. congruently melting systems.
- III. Distribution of acetic/ benzoic acid between water and chloroform or cyclohexane.
- IV. Study the equilibrium of at least one of the following reactions by the distribution method:
 - (i) $\text{I}_2(\text{aq}) + \text{I}^-(\text{aq}) \rightarrow \text{I}_3^-(\text{aq})$
 - (ii) $\text{Cu}^{2+}(\text{aq}) + n\text{NH}_3 \rightarrow \text{Cu}(\text{NH}_3)_n^{2+}$

Potentiometry:

- V. Perform the following potentiometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Dibasic acid vs. strong base iv. Potassium dichromate vs. Mohr's salt

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011). 25
 - Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
 - Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).
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SEMESTER IV

CHEMISTRY - C VIII: *INORGANIC CHEMISTRY III* (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Coordination Chemistry:

Werner's theory, valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of $10 Dq$ (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of $10 Dq$ (Δ_o , Δ_t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect, polynuclear complexes, Labile and inert complexes.

(26 Lectures)

Transition Elements:

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams) Different between the first, second and third transition series.

Chemistry of Cr, Mn, Fe and Co in various oxidation states with special reference to the following compounds: peroxo compounds of chromium, potassium dichromate, potassium

permanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite.

(14 Lectures)

Lanthanoids and Actinoids:

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

(6 Lectures)

Inorganic Reaction Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect. Thermodynamic and Kinetic stability.

(14 Lectures)

Reference Books:

- Purcell, K.F & Kotz, J.C., *Inorganic Chemistry* W.B. Saunders Co, 1977.
- Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
- Cotton, F.A. & Wilkinson, G., *Advanced Inorganic Chemistry* Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley & Sons, NY, 1967.
- Greenwood, N.N. & Earnshaw A., *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
- Miessler, G. L. & Tarr, Donald A. *Inorganic Chemistry 3rd Ed.(adapted)*, Pearson, 2009

Practical C – VIII Lab: 60 Lectures

Gravimetric Analysis:

- Estimation of nickel (II) using Dimethylglyoxime (DMG).
- Estimation of copper as CuSCN
- Estimation of iron as Fe₂O₃ by precipitating iron as Fe(OH)₃.
- Estimation of Al(III) by precipitating with oxine and weighing as Al(oxine)₃ (aluminium oxinate).

Inorganic Preparations:

- Tetraamminecopper (II) sulphate, [Cu(NH₃)₄]SO₄.H₂O
- Acetylacetonate complexes of Cu²⁺/Fe³⁺
- Tetraamminecarbonatocobalt (III) nitrate
- Potassium tri(oxalato)ferrate(III)

Properties of Complexes

- Measurement of 10 Dq by spectrophotometric method
- Verification of spectrochemical series.
- Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetonate, DMG, glycine) by substitution method.

Reference Book:

- Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.
 - G. Marr and B.W. Rockett, *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972
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CHEMISTRY - C IX: ORGANIC CHEMISTRY III

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Nitrogen Containing Functional Groups

Preparation and important reactions of nitro compounds, nitriles and isonitriles.

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

Diazonium Salts: Preparation and their synthetic applications.

(18 Lectures)

Polynuclear Hydrocarbons

Aromaticity of polynuclear hydrocarbons, structure elucidation of naphthalene; Preparation and properties of naphthalene, phenanthrene and anthracene.

(8 Lectures)

Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Indole (Fischer indole synthesis and Madelung synthesis), Quinoline and isoquinoline, (Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction)

(22 Lectures)

Alkaloids

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

(6 Lectures)

Terpenes

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

(6 Lectures)

Reference Books:

•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: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly& Sons (1976).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiParakashan (2010).

Practical C – IX Lab: 60 Lectures

- 1.Functional group test for nitro, amine and amide groups.
- 2.Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols , carbonyl compounds and esters)

Reference Books:

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

CHEMISTRY - C X: PHYSICAL CHEMISTRY IV (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Conductance: Quantitative aspects of Faraday's laws of electrolysis Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at 29 infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules. Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

(18 Lectures)

Chemical Kinetics: Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates. **(22 Lectures)**

Catalysis: Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis. **(8 Lectures)**

Photochemistry: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence. **(12 Lectures)**

Reference Books:

- Atkins, P.W & Paula, J.D. Physical Chemistry, 9th Ed., Oxford University Press (2011).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Barrow, G. M., Physical Chemistry 5th Ed., Tata McGraw Hill: New Delhi (2006).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Rogers, D. W. Concise Physical Chemistry Wiley (2010).
- Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed., John Wiley & Sons, Inc. (2005).

Practical C – X Lab: 60 Lectures

Conductometry:

- I. Determination of cell constant
- II. Determination of conductivity, molar conductivity, degree of dissociation and dissociation constant of a weak acid.
- III. Perform the following conductometric titrations: i. Strong acid vs. strong base ii. Weak acid vs. strong base iii. Mixture of strong acid and weak acid vs. strong base iv. Strong acid vs. weak base

Chemical Kinetics:

- IV. Study the kinetics of the following reactions.
1. Iodide-persulphate reaction (i) Initial rate method; (ii) Integrated rate method
 2. Acid hydrolysis of methyl acetate with hydrochloric acid.
 3. Saponification of ethyl acetate.
 4. Comparison of the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate.

Reference Books:

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

CHEMISTRY - C XI: *ORGANIC CHEMISTRY IV* (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides;

Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine;
Structure of polynucleotides (DNA and RNA).

(9 Lectures)

Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

α -Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pK_a values, isoelectric point and electrophoresis;

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

(18 Lectures)

Enzymes

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

Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance.

(6 Lectures)

Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity.

(8 Lectures)

Concept of Energy in Biosystems

Cells obtain energy by the oxidation of foodstuff (organic molecules). Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD⁺, FAD.

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

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

(7 Lectures)

Pharmaceutical Compounds: Structure and Importance

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

(12 Lectures)

Reference Books:

•Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) Biochemistry. VIth Edition. W.H. Freeman and Co.

•Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.

•Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. XXVIII edition. Lange Medical Books/ McGraw-Hill.

Practical C – XI Lab: 60 Lectures

1. Estimation of glycine by Sorenson's formalin method.
2. Study of the titration curve of glycine.
3. Estimation of proteins by Lowry's method.
4. Study of the action of salivary amylase on starch at optimum conditions.
5. Effect of temperature on the action of salivary amylase.
6. Saponification value of an oil or a fat.
7. Determination of Iodine number of an oil/ fat.
8. Isolation and characterization of DNA from onion/ cauliflower/peas.

Reference Books:

- Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
 - Arthur, I. V. Quantitative Organic Analysis, Pearson.
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CHEMISTRY - C XII: PHYSICAL CHEMISTRY V (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

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

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

Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar (Derivation not required). Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).

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

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+ . Bonding and antibonding orbitals. Qualitative extension to H_2 . Comparison of LCAO-MO and VB treatments of H_2 (only wave functions, detailed solution not

required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH).

(30 Lectures)

Molecular Spectroscopy: Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation.

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

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

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

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

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

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

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

(30 Lectures)

Reference Books:

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

- Kakkar, R. Atomic & Molecular Spectroscopy, Cambridge University Press (2015).

Practical C – XII Lab: 60 Lectures

Colorimetry :

- I. Verify Lambert-Beer's law and determine the concentration of $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ in a solution of unknown concentration
- II. Determine the concentrations of KMnO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ in a mixture.
- III. Study the kinetics of iodination of propanone in acidic medium.
- IV. Determine the amount of iron present in a sample using 1, 10-phenanthroline.
- V. Determine the dissociation constant of an indicator (phenolphthalein).
- VI. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.
- VII. Analysis of the given vibration-rotation spectrum of $\text{HCl}(\text{g})$

Adsorption

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

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.

Reference Books:

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

CHEMISTRY - C XIII: *INORGANIC CHEMISTRY IV* **(Credits: Theory-04, Practicals-02)**

Theory: 60 Lectures

Theoretical Principles in Qualitative Analysis (H₂S Scheme)

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

(12 Lectures)

Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π -acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

(26 Lectures)

Bioinorganic Chemistry:

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents in medicine, Cisplatin as an anti-cancer drug.

Iron and its application in bio-systems, Haemoglobin, Myoglobin; Storage and transfer of iron.

(14 Lectures)

Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Synthetic gasoline (Fischer Tropsch reaction)
3. Polymerisation of ethene using Ziegler-Natta catalyst

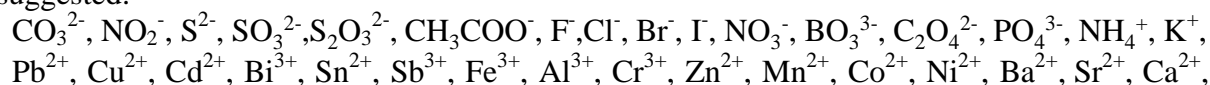
(8 Lectures)

Reference Books:

- Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972
- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996-03-07.
- Lippard, S.J. & Berg, J.M., *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.
- Cotton, F.A., Wilkinson, G., & Gaus, P.L. *Basic Inorganic Chemistry 3rd Ed.*; Wiley India,
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed.*, Harper Collins 1993, Pearson, 2006.
- Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry 3rd Ed.*, John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements 2nd Ed*, Elsevier, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. *Concise Inorganic Chemistry 5th Ed.*, John Wiley and sons 2008.
- Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.
- Shriver, D.D., Atkins, P. and Langford, C.H., *Inorganic Chemistry 2nd Ed.*, Oxford University Press, 1994.
- Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977
- Miessler, G. L. & Tarr, Donald A., *Inorganic Chemistry 4th Ed.*, Pearson, 2010.
- Collman, James P. et al. *Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.
- Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. John Wiley New York, NY, 2000.
- Spessard, Gary O., & Miessler, Gary L., *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

Practical C – XIII Lab: 60 Lectures

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





Mixtures should preferably contain one interfering anion, **or** insoluble component (BaSO₄, SrSO₄, PbSO₄, CaF₂ or Al₂O₃) **or** combination of anions e.g. CO₃²⁻ and SO₃²⁻, NO₂⁻ and NO₃⁻,

Cl⁻ and Br⁻, Cl⁻ and I⁻, Br⁻ and I⁻, NO₃⁻ and Br⁻, NO₃⁻ and I⁻.

Spot tests should be done whenever possible.

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

- i. Ni (II) and Co (II)
- ii. Cu(II) and Cd(II)

Reference Books:

- *Vogel's Qualitative Inorganic Analysis*, Revised by G. Svehla.
 - Vogel, A.I. *A Textbook of Quantitative Analysis*, ELBS. 1986
-

CHEMISTRY - C XIV: ORGANIC CHEMISTRY V (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures Organic Spectroscopy

General principles Introduction to absorption and emission spectroscopy.

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

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

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

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

(24 Lectures)

Carbohydrates

Occurrence, classification and their biological importance.

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

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

(16 Lectures)

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing;

Synthesis and applications of: Azo dyes – Methyl orange; Triphenyl methane dyes - Malachite green and Rosaniline ; Phthalein Dyes – Phenolphthalein; Natural dyes – structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

(8 Lectures)

Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers;

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

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

(12 Lectures)

Reference Books:

- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
- Gowariker, V. R.; Viswanathan, N. V. &Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.

- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PrajatiPrakashan (2010).
- Kemp, W. Organic Spectroscopy, Palgrave

Practical C – XIV Lab: 60 Lectures

- 1.Extraction of caffeine from tea leaves.
- 2.Preparation of urea formaldehyde resin.
- 3.Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, e.g. salicylic acid, cinnamic acid, nitrophenols etc.
- 4.Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).
- 5.Preparation of methyl orange.

Reference Books:

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

CHEMISTRY-DSE 1 : Choose any one of the following:

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.

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:

- Atkins, Peter, Overton, Tina, Rourke, Jonathan, Weller, Mark and Armstrong, Fraser
Shriver & Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press 2011-2012
- Adam, D.M. *Inorganic Solids: An introduction to concepts in solid-state structural chemistry*, John Wiley and Sons, London, New York, Sydney, Toronto, 1974
- Poole Jr., Charles P., Owens, Frank J., *Introduction to Nanotechnology* John Wiley and Sons, 2003.

CHEMISTRY PRACTICAL - DSE LAB: NOVEL INORGANIC SOLIDS

60 Lectures

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

Reference Book:

- Fahlman, B.D., *Materials Chemistry*, Springer, 2007

CHEMISTRY-DSE: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures
(Compulsory elective)

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: Brief introduction to types of ceramics. Superconducting and semiconducting oxides, fullerenes, carbon nanotubes and carbon fibre.

Cements: Manufacture of cement and the setting process, quick setting cements.

(16 Lectures)

Fertilizers:

Different types of fertilizers (N, P and K). Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates, superphosphate of lime.

(8 Lectures)

Surface Coatings:

Brief introduction to and classification of surface coatings. Paints and pigments - formulation, composition and related properties. Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

(4 Lectures)

Batteries:

Working of the following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

(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.

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.

(6 Lectures)

Reference Books:

- Stocchi, E., *Industrial Chemistry*, Vol I, Ellis Horwood Ltd. UK, 1990
- Felder, R. M. and Rousseau, R.W., *Elementary Principles of Chemical Processes*, Wiley

- Publishers, New Delhi, 2005.
- Kingery, W. D., Bowen H. K. and Uhlmann, D. R. *Introduction to Ceramics*, Wiley Publishers, New Delhi, 1976.
 - Kent, J. A. (ed) *Riegel's Handbook of Industrial Chemistry*, 9th Ed., CBS Publishers, New Delhi, 1997
 - Jain, P. C. and Jain, M. *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi 2005
 - Gopalan, R., Venkappayya, D. and Nagarajan, S. *Engineering Chemistry*, Vikas Publications, New Delhi, 2004.
 - Sharma, B. K. *Engineering Chemistry*, Goel Publishing House, Meerut, 2006
-

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:

- Stocchi, E., *Industrial Chemistry*, Vol I, Ellis Horwood Ltd. UK, 1990
 - Felder, R. M. and Rousseau, R.W., *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi, 2005.
 - Kingery, W. D., Bowen H. K. and Uhlmann, D. R. *Introduction to Ceramics*, Wiley Publishers, New Delhi, 1976.
 - Kent, J. A. (ed) *Riegel's Handbook of Industrial Chemistry*, 9th Ed., CBS Publishers, New Delhi, 1997
 - Jain, P. C. and Jain, M. *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 - Gopalan, R., Venkappayya, D. and Nagarajan, S. *Engineering Chemistry*, Vikas Publications, New Delhi, 2004.
 - Sharma, B. K. *Engineering Chemistry*, Goel Publishing House, Meerut, 2006
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CHEMISTRY-DSE 2-4 : Choose any three of the following:

CHEMISTRY-DSE: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

- **Basic Computer system (in brief)**-Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High Level languages (Machine language, Assembly language; QBASIC, FORTRAN and C++); Software Products (Office, chemsketch, scilab, matlab, hyperchem, etc.), internet application. **(5 Lecture)**
- **Use of Programming Language for solving problems in Chemistry**
Computer Programming Language- QBASIC, (for solving some of the basic and in turn complicated chemistry problems). QB4 version of QBASIC can be used.

Programming Language – QBASIC; Commands: INPUT and PRINT Commands; GOTO, If, ELSEIF, THEN and END IF Commands; FOR and NEXT Commands; Library Functions (ABS, ASC, CHR\$, EXP,INT, LOG, RND, SQR, TAB and trigonometric Functions), DIM, READ, DATA, REM, RESTORE, DEF FNR, GOSUB, RETURN, SCREEN, VIEW, WINDOW, LINE, CIRCLE. LOCATE, PSET Commands.

Simple programs using above mentioned commands.

QBASIC programs for Chemistry problems - Example: plotting van der Waal Isotherms (Simple Problem, available in general text books) and observe whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation and calculation of area under the curves (Complicated Problem, not available in general text books).

Solution of quadratic equation, polynomial equations (formula, iteration and Newton – Raphson methods, binary bisection and Regula Falsi); Numerical differential, Numerical integration (Trapezoidal rule), Simultaneous equations, Matrix addition and multiplication, Statistical analysis.

(40 Lecture)

- **Use of Software Products**

Computer Software like Scilab, Excel, etc to solve some of the plotting or calculation problems.

Basic idea of Molecular Modelling using software like chemsketch, arguslab and Accelrys JDraw etc for geometry optimization and potential energy surface (local and global minima) **(15 lecture)**

Practical: 60 Periods

- **Computer programs using QBASIC based on numerical methods**

1. Roots of equations: (e.g. volume of gas using van der Waals equation 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).
4. Probability distributions (gas kinetic theory) and mean values.
5. Matrix operations.
6. Graphic programs related to Chemistry problems. *e.g.* van der Waals isotherm, Compressibility versus pressure curves, Maxwell distribution curves, concentration-time graph, pH metric titration curve, conductometric titration curves, Lambert Beer's law graph, s, p, d orbital shapes, radial distribution curves, etc.

- **Use of Software Products**

1. Computer Software like Scilab and Excel, etc for data handling and manipulation.
2. Simple exercises using molecular visualization software like Chems sketch, Arguslab and Accelrys JDraw, geometry optimization and potential energy surface of molecules like carbon dioxide, water, ethane, cyclohexane and benzene (local and global minima)

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). -----

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 of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Optical methods of analysis:(5 Lectures)

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

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

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers.

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 non-aqueous media.

Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods.

(15 Lectures)

Reference Books:

- Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others)* 5th Ed. The English Language Book Society of Longman .
- Willard, Hobart 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, 1998.
- Mikes, O. and Chalmers, R.A. Ed. *Laboratory Hand Book of Chromatographic and Allied Methods*, Elles Horwood Ltd. London.
- Dilts, R.V. *Analytical Chemistry – Methods of separation* Van Nostrand 1974.

PRACTICALS-DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

60 Lectures

I. Separation Techniques

Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Co^{2+} and Ni^{2+} .

(ii) Separation and identification of the amino acids present in the given mixture by paper chromatography. Reporting the R_f values.

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.

Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium

(iv) Qualitative detection of nitrate, phosphate

Ion exchange:

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

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

III Spectrophotometry

Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO_4 , KMnO_4)

Reference Books:

- Vogel, Arthur I: *A Text book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Willard, Hobart 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, 1998.
- Mikes, O. & Chalmers, R.A. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Horwood Ltd. London.

- Dilts, R.V. *Analytical Chemistry – Methods of separation* Van Nostrand 1974
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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.

46

(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: MOLECULAR MODELLING & DRUG DESIGN

60 Lectures

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

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

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: 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. Bifunctional 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

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:

- Malcolm 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 special emphasis on the following with 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, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
- Prevention/ minimization of hazardous/ toxic products reducing toxicity
risk = (function) hazard x exposure ; waste or pollution prevention hierarchy
- Green solvents– super critical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents
- Energy requirements for reactions – alternative sources of energy: use of microwaves

and ultrasonic energy

- Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups;
- use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, bio catalysis, asymmetric catalysis and photo catalysis.
- Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
- Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

(30 Lectures)

Examples of Green Synthesis/ Reactions and some real world cases

1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
4. Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
7. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
8. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils
9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

(16 Lectures)

Future Trends in Green Chemistry

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

(10 Lecture)

Reference Books:

- Ahluwalia, V.K. and Kidwai, M.R. *New Trends in Green Chemistry*, Anamalaya Publishers, 2005
 - Anastas, P.T. and Warner, J.K. *Oxford Green Chemistry -Theory and Practical*, University Press, 1998
 - Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker, 2001
 - Cann, M.C. and Connely, M.E. *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
 - Ryan, M.A. and Tinnesand, M., *Introduction to Green Chemistry*, American Chemical Society Washington, 2002
 - Lancaster, Mike, *Green Chemistry an Introductory Text* 2nd Ed., RSC Publishing,. ISBN: 978-1-84755-873-2
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CHEMISTRY PRACTICAL - DSE LAB: GREEN CHEMISTRY

60 Lectures

1. Safer starting materials

Preparation and characterization of nano particles of gold using tea leaves.

1. Using renewable resources

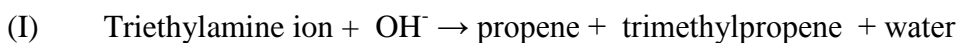
Preparation and characterization of biodiesel from vegetable oil/ waste cooking oil

3. Avoiding waste

Principle of atom economy.

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

Preparation of propene by two methods can be studied



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

6. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

Alternative sources of energy

8. Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).

9. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

Reference Books:

- Anastas, P.T and Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press, 1998
- Kirchoff, M. and 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. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph*, I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
- Cann, M.C. and Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society, 2008
- Cann, M. C. and Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society, 2008
- Lancaster, Mike *Green Chemistry: An introductory text: 2nd Ed.* RSC publishing, ISBN 978-1-84755-873-2
- Pavia, D.L., Kriz, G.S., Lampman, G.M. and Engels, R.G. *Introduction to Organic Laboratory Techniques – a Microscale Approach* 4th Ed., Brooks-Cole Laboratory Series for Organic Chemistry, 2006

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).

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 (AgNO₃ and potassium chromate).
6. Estimation of total alkalinity of water samples (CO₃²⁻, HCO₃⁻) using double titration method.
7. Measurement of dissolved CO₂.
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: 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.

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.

Skill Enhancement Course (any four) (Credit: 02 each)- SEC1 to SEC4

IT SKILLS FOR CHEMISTS (Credits: 02)

(Hands on Exercises: 60 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, pKa 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 Ftest.

Presentation: Presentation graphics

Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3 Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2 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) **(Hands on Exercises: 60 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.

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

Paper chromatographic separation of mixture of metal ion (Ni^{2+} and Co^{2+}).

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).

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, 1988.
2. Skoog, D.A. and Leary, J.J., *Instrumental Methods of Analysis*, Saunders College Publications, New York, 1992
3. Skoog, D.A.; West, D.M. and Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth, 1992
4. Harris, D. C. *Quantitative Chemical Analysis 7th Ed.*, W. H. Freeman and Co., New York, 2007
5. Dean, J. A. *Analytical Chemistry Handbook*, McGraw Hill, 2007
6. Day, R. A. and Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India, 1991

7. Freifelder, D. *Physical Biochemistry 2nd Ed.*, W.H. Freeman and Co., N.Y. 1982
 8. Cooper, T.G. (Ed.) *The Tools of Biochemistry*, John Wiley and Sons, N.Y. 1977
 9. Svehla, G., *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall, 1996
 10. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M.J.K., *Vogel's Quantitative Chemical Analysis 6th Ed.*, Prentice Hall, 2007.
 11. Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York, 1995
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CHEMICAL TECHNOLOGY & SOCIETY (Credits: 02)

(Hands on Exercises: 60 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:

John W. Hill, Terry W. McCreary & Doris K. Kolb, Chemistry for changing times 13th Ed.

CHEMOINFORMATICS (Credits: 02)

(Hands on Exercises: 60 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.

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.

References:

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, TataMcGraw-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)

(Hands on Exercises: 60 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 β and -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.
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GREEN METHODS IN CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 Lectures)

Theory and Hands-on Experiments

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents, Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

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

- 1 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- 2 Designing of Environmentally safe marine antifoulant.
- 3 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- 4 An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

PRACTICALS

- 1 Preparation and characterization of biodiesel from vegetable oil.
- 2 Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.
- 3 Mechanochemical solvent free synthesis of azomethine.

- 4 Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper(II)

Reference Books:

1. Anastas, P.T. and Warner, J.K. *Oxford Green Chemistry- Theory and Practical*, University Press, 1998
2. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker, 2001
3. Cann, M.C. and Connely, M.E., *Real-World Cases in Green Chemistry*, American Chemical Society, Washington, 2000
4. Ryan, M.A. and Tinnesand, M., *Introduction to Green Chemistry*, American Chemical Society, Washington, 2002
5. Sharma, R.K., Sidhwani, I.T. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph*, I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
6. Lancaster, Mike *Green Chemistry: An Introductory Text 2nd Ed.*, RSC Publishing, ISBN 978-1-84755-873-2, 2010
7. Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated “ A social Awareness Project”
Indu Tucker Sidhwani, Geeta Saini, Sushmita Chowdhury, Dimple Garg, Malovika, Nidhi Garg, Delhi University Journal of Undergraduate Research and Innovation, Vol1, Issue 1, Feb 2015. ISSN: 2395-2334.

PHARMACEUTICAL CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 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)

(Hands on Exercises: 60 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.

PESTICIDE CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 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

1To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.

2Preparation of simple organophosphates, phosphonates and thiophosphates

Reference Book:

•R. Cremllyn: Pesticides, John Wiley.

FUEL CHEMISTRY (Credits: 02)

(Hands on Exercises: 60 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, pour 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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**Generic Elective Papers (GE) (Minor-Chemistry) (any four) for other Departments/Disciplines:
(Credit: 06 each)**

**ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC
(Credits: Theory-4, Practicals-2)**

**THEORY Lectures: 60
Section A: Inorganic Chemistry-1 (30 Periods)**

Atomic Structure: Review of: Bohr's theory and its limitations, Heisenberg Uncertainty principle.

Dual behaviour of matter and radiation, de-Broglie's relation. 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 (no derivation), 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 (H_2O , NH_3 , PCl_5 , SF_6 , ClF_3 , SF_4) 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^+ .

(16 Lectures)

Section B: Organic Chemistry-I (30 Lectures)

Fundamentals of Organic Chemistry

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

Reaction intermediates: Carbocations, Carbanions and free radicals. Electrophiles and nucleophiles

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 physical property & chemical reactions) to be studied with mechanism in context to their structure.

Alkanes: *Preparation:* Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, Grignard reagent. *Reactions:* Free radical Substitution: Halogenation.

Alkenes: *Preparation:* Elimination reactions: Dehydration of alcohols and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO_4) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymercuration-demercuration, Hydroboration-oxidation.

Alkynes: *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 and acidity of alkynes, addition of bromine and alkaline KMnO_4 , ozonolysis and oxidation with hot alk. KMnO_4 . Hydration to form carbonyl compounds

(12 Lectures)

Reference Books:

- J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.17
- F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
- Douglas, McDaniel and Alexander: *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
- Atkins, Overton, Rourke, Weller, Armstrong, Shriver and Atkins *Inorganic Chemistry*, Oxford

CHEMISTRY 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. Purification of OC by crystallisation (from water and alcohol) and distillation.
2. Criteria of purity: Determination of Mpt/Bpt
3. Detection of extra elements (N, S, Cl, Br, I) in organic compounds
4. 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.
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CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY I

(Credits: Theory-4, Practicals-2)

THEORY: Lectures: 60

Section A: Physical Chemistry-1 (30 Lectures)

Chemical Energetics

Review of thermodynamics and the Laws of Thermodynamics.

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

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

(10 Lectures)

Chemical Equilibrium:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between G and G° , 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 physical properties and Chemical reactions) to be studied in context to their structure with mechanism.

Aromatic hydrocarbons

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

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

(8 Lectures)

Alkyl and Aryl Halides

Alkyl Halides .

Preparation: from alkenes and alcohols.

Reactions: Types of Nucleophilic Substitution (S_N1 , S_N2 and S_Ni) 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 electrophilic and nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$).

Relative reactivity of alkyl, allyl, benzyl, vinyl and aryl halides towards Nucleophilic substitution reactions. .

(8 Lectures)

Alcohols, Phenols and Ethers)

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

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3), factors affecting acidity, Oppeneauer oxidation

Diols: 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. acidity and factors affecting

Ethers (aliphatic and aromatic).

Preparation : Williamson ether synthesis.

Reactions: Cleavage of ethers with HI

Aldehydes and ketones (aliphatic and aromatic):

Preparation: from acid chlorides and from nitriles.

Reactions – Nucleophilic addition, Nucleophilic addition – elimination reaction including 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 Lening 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: 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 (KNO₃, NH₄Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of *H*.

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. 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

2. Systematic Qualitative organic analyses of organic compounds possessing monofunctional groups (Alcohols, Phenols, Carbonyl, -COOH) and preparation of one suitable derivative.

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.

SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY-II

(Credits: Theory-4, Practicals-2)

THEORY: Lectures: 60

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, FeCl₃-H₂O and Na-K only).

Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions.

Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only 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: G , H and S from EMF data.

Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge.

pH determination using hydrogen electrode and quinhydrone electrode.

Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).

Section B: Organic Chemistry-3 (30 Lectures)

Functional group approach for the following reactions (preparations Physical Property & Chemical reactions) to be studied in context to their structure with mechanism.

Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic)

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Vohlard - Zelinsky Reaction, Acidity of carboxylic acid, effect of substitution on acid strength.

Carboxylic acid derivatives (aliphatic):

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

Reactions: Relative reactivities of acid derivatives towards nucleophiles, Reformatsky Reaction,
Perkin condensation.

(6 Lectures)

Amines and Diazonium Salts

Amines (Aliphatic and Aromatic):

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

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

Diazonium salts: *Preparation:* from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

(6 Lectures)

Amino Acids, Peptides and Proteins:

Zwitterion, Isoelectric point and Electrophoresis

Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis.

Reactions of Amino acids: ester of $-\text{COOH}$ group, acetylation of $-\text{NH}_2$ 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
disaccharides (sucrose, cellobiose, maltose, lactose) and polysaccharides (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

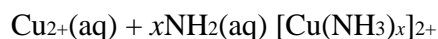
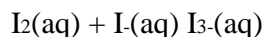
CHEMISTRY LAB: SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & BIOMOLECULES

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

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

Section B: Organic Chemistry

I Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (amide, nitro, amines, Hydrocarbons, Halo Hydrocarbons) and preparation of one derivative.

II

1. Determination of the concentration of glycine solution by formylation method
2. Action of salivary amylase on starch
3. Differentiation between a reducing and 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.

CHEMISTRY OF S- AND P-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS (Credits: Theory-4, Practicals-2)

THEORY: Lectures: 60

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 with reference to cyanide process for silver and gold, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, 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

Diborane and concept of multicentre bonding

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

Hydrides of nitrogen (NH_3 , N_2H_4 , N_3H , NH_2OH) 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 Lening 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.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 3rd Ed.(adapted)*, Pearson, 2009 ISBN 978-81-31718858.

CHEMISTRY LAB: CHEMISTRY OF s- AND p-BLOCK ELEMENTS, STATES OF MATTER & CHEMICAL KINETICS

60 Lectures

Section A: Inorganic Chemistry

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

Cations : NH₄⁺, Pb²⁺, Bi³⁺, Cu²⁺, Fe³⁺, Al³⁺, Co²⁺, Ni²⁺, Mn²⁺, Zn²⁺, Ba²⁺, Sr²⁺, Ca²⁺, K⁺
Anions : CO₃²⁻, S²⁻, SO₃²⁻, 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.

GE: 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.

GE 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. Determination of the composition of the Fe^{3+} - salicylic acid complex / Fe^{2+} - phenanthroline complex in solution by Job's method.

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.

Colorimetry

- 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 $\text{HCl}(\text{g})$

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.
-

GE: 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 Cu.

A study of the following compounds (including preparation and important properties);

Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, $K_3[Fe(CN)_6]$, 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, Zeise's salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. π -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 iron in oxygen transport, haemoglobin, myoglobin, storage and transport of iron.

(12 Lectures)

Section B: Organic Chemistry-4 (30 Lectures) Polynuclear and heteronuclear aromatic compounds:

Structure elucidation of naphthalene, preparation and properties of naphthalene and anthracene. Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Furan, Pyrrole, Thiophene, and Pyridine.

(12 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).

(12 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.

GE 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

LiCl₃.

Section B: Organic Chemistry

Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, alcoholic, phenolic, carbohydrates, 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).
-

GE: 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 (tbutyloxycarbonyl 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.

Reference Book:

- 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.

GE 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 synthesize aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Reference Books:

- 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.
-

References Books:

Inorganic Chemistry

- Lee, J. D., *A New Concise Inorganic Chemistry*, ELBS, 1991
- Atkins, Peter, Overton, Tina, Rourke, Jonathan, Weller, Mark and Armstrong, Fraser
Shriver & Atkins' Inorganic Chemistry, 5th Edition, Oxford University Press 2011-2012

Physical Chemistry

- Chang, Raymond, *Physical Chemistry*, McGraw-Hill Publishing Company, 2006
- Kapoor, K.L., *A Textbook of Physical Chemistry Vol. 1, 5e*, Tata McGraw-Hill Publishing Company, 2014
- Kapoor, K.L. *A Textbook of Physical Chemistry Vol. 2*, McGraw-Hill Education, 2014
- Kapoor, K.L., *A Textbook of Physical Chemistry Vol. 3, 4e*, McGraw-Hill Education 2014
- Kapoor, K.L., *A Textbook of Physical Chemistry Vol. 4, 5e*, McGraw Hill Education 2014
- Barrow, Gordon M., *Physical Chemistry 6e* McGraw-Hill Education, 1996
- Levine, Ira N., *Physical Chemistry 6e*, McGraw-Hill Education, 2008

Organic Chemistry

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