CHOICE BASED CREDIT SYSTEM B. Sc. HONOURS WITH CHEMISTRY

B.Sc. (H) ChemistryThree Year Course of Study(2019-2022)

Course Structure

Details of courses	***Credits** Theory+ Practical	Theory+Tutorial
I. Core Course (14 Papers)	14×4= 56	14×5=70
Core Course Practical (14 Papers)	14×2=28	14×1=14
II. Elective Course (8 Papers)		
A.1. Discipline Specific Elective **(4 Papers)**	4×4=16	4×5=20
A.2. Discipline Specific Elective Practical **(4 Papers)**	4×2=8	4×1=4
B.1. Generic Elective/ Interdisciplinary **(4 Papers)**	4×4=16	4×5=20
B.2. Generic Elective Practical **(4 Papers)**	4×2=8	4×1=4
III. Ability Enhancement Courses		
1. **Ability Enhancement Compulsory (2 Papers of 4 credit each)** Environmental Science English/MIL Communication	4×2=8	4×2=8
2. **Ability Enhancement Elective** (Skill Based) (Minimum 2) **(2 Papers of 4 credit each)**	4×2=8	4×2=8

Total credits =148

Semester	CORE COURSE (14)	Ability Enhancement Compulsory Course (AECC) (2)	Ability Enhancement Elective Course (AEEC) (2) (Skill Based)	Elective: Discipline Specific DSE(4)	Elective: Generic (GE) (4)
I	Inorganic I: Atomic Structure & Chemical Bonding-I (4+4) Physical I: States of Matter & Ionic Equilibrium (4+4)	(English Communication/ MIL) /Environmental Science			GE-1
II	Organic I:Basics & Hydrocarbons (4+4) Physical II: Chemical Thermodynamics & its Applications (4+4)	Environmental Science/ (English/MIL Communication)			GE-2
III	Inorganic II: s- and p-Block Elements (4+4) Organic II: Oxygen Containing Functional Groups (4+4) Physical III: Phase Equilibria & Chemical Kinetics (4+4)		SEC-I		GE-3
IV	Inorganic III: Coordination Chemistry (4+4) Organic III: Heterocyclic Chemistry (4+4) Physical IV: Electrochemistry (4+4)		SEC-2		GE-4
V	Organic IV: Biomolecules (4+4) Physical V: Quantum Chemistry & Spectroscopy(4+4)			DSE-1 DSE-2	
VI	Inorganic IV: Organometallic Chemistry (4+4) Organic Chemistry V: Spectroscopy (4+4)			DSE-3 DSE-4	

S.N	Code	Course Name	Category	L-T-P	Credits
SEMESTER I					
1	**ES101**	Environmental Science	AECC 1	4-0-0	4
2	**CHH101**	Inorganic Chemistry-I	Core Course-I	4-0-0	4
3	**CHH103**	Inorganic Chemistry Lab-I	Core Course-I Practical	0-0-4	2
4	**CHH105**	Physical Chemistry-I	Core Course-II	4-0-0	4
5	**CHH107**	Physical Chemistry Lab-I	Core Course-II Practical	0-0-4	2
6		*GE-1	Generic Elective -1	4-0-0 5-0-0	4/5
7			Generic Elective -1 Practical/Tutorial	0-0-4 0-1-0	2/1
				21-1-12	
		Total Contact Hour		**34**	
		Total Credits			**22/22**
SEMESTER II					
1	**EN105**	Communicative English	AECC 2	4-0-0	4
2	**CHH102**	Organic Chemistry-I	Core Course-III	4-0-0	4
3	**CHH104**	Organic Chemistry Lab-I	Core Course-III Practical	0-0-4	2
4	**CHH106**	Physical Chemistry-II	Core Course-IV	4-0-0	4
5	**CHH108**	Physical Chemistry Lab-I	Core Course-IV Practical	0-0-4	2
6		*GE-2	Generic Elective -2	4-0-0 5-0-0	4/5
7			Generic Elective -2 Practical/Tutorial	0-0-4 0-1-0	2/1
		Total		21-1-12	**22/22**
		Total Contact Hour		**34**	
SEMESTER III					
1	**CHH201**	Inorganic Chemistry-II	Core Course-V	4-0-0	4
2	**CHH203**	Inorganic Chemistry Lab-II	Core Course-V Practical	0-0-4	2
3	**CHH205**	Organic Chemistry-II	Core Course-VI	4-0-0	4
4	**CHH207**	Organic Chemistry Lab-II	Core Course-VI Practical	0-0-4	2
5	**CHH209**	Physical Chemistry-III	Core Course-VII	4-0-0	4
6	**CHH211**	Physical Chemistry Lab-III	Core Course-VII Practical	0-0-4	2
7	**CHH213**	Intellectual Property Rights	Skill Enhancement Course -1	4-0-0	4
8		*GE-3	Generic Elective -3	4-0-0 5-0-0	4/5
9			Generic Elective -3 Practical/Tutorial	0-0-4 0-1-0	2/1
		Total		**25-1-16**	**28/28**
		Total Contact Hour		**42**	
SEMESTER IV					
1	**CHH202**	Inorganic Chemistry III	Core Course VIII	4-0-0	4
2	**CHH204**	Inorganic Chemistry Lab III -	Course VIII Practical	0-0-4	2
3	**CHH206**	Organic Chemistry III	Core Course IX	4-0-0	4

4	**CHH208**	Organic Chemistry Lab- III	Course IX Practical	0-0-4	2
5	**CHH210**	Physical Chemistry IV	Core Course X	4-0-0	4
6	**CHH212**	Physical Chemistry Lab- IV	Course X Practical	0-0-4	2
7	**CHH214**	Pharmaceutical Chemistry	Skill Enhancement Course-2	4-0-0	4
8		*GE-4	Generic Elective-4	4-0-0 5-0-0	4/5
9			Generic Elective-4 Practical	0-0-4 0-1-0	2/1
		Total		**25-1-16**	**28/28**
		Total Contact Hour		**42**	
SEMESTER V					
1	**CHH301**	Organic Chemistry IV	Core Course XI	4-0-0	4
2	**CHH303**	Organic Chemistry Lab- IV	Core Course XI Practical	0-0-4	2
3	**CHH305**	Physical Chemistry V	Core Course XII	4-0-0	4
4	**CHH307**	Physical Chemistry Lab- V	Core Course XII Practical	0-0-4	2
5	**Refer Table1**	DSE-1	Discipline Specific Elective -1	4-0-0	4
6	**Refer Table1**	DSE-1 Lab	Discipline Specific Elective -1 Practical	0-0-4	2
7	**Refer Table1**	DSE-2	Discipline Specific Elective -2	4-0-0	4
8	**Refer Table1**	DSE-2 Lab	Discipline Specific Elective -2 Practical	0-0-4	2
		Total		**16-0-16**	**24**
		Total Contact Hour		**32**	
SEMESTER VI					
1	**CHH302**	Inorganic Chemistry IV	Core Course XIII	4-0-0	4
2	**CHH304**	Inorganic Chemistry Lab- IV	Core Course XIII Practical	0-0-4	2
3	**CHH306**	Organic Chemistry V	Core Course XIV	4-0-0	4
4	**CHH308**	Organic Chemistry Lab- V	Core Course XIV Practical	0-0-4	2
5	**Refer Table1**	DSE-3	Discipline Specific Elective -3	4-0-0	4
6	**Refer Table1**	DSE-3 Lab	Discipline Specific Elective -3 Practical	0-0-4	2
7	**Refer Table1**	DSE-4	Discipline Specific Elective -4	4-0-0	4
8	**Refer Table1**	DSE-4 Lab	Discipline Specific Elective -4 Practical	0-0-4	2
				16-0-16	**24**
		Total Contact Hour		**32**	
		Total Credit			**148**

Table 1: Discipline Specific Elective Papers: (Credit: 06 each)

Semester	Course Code	Course Name	Category	L-T-P	Credits
	Select any one DSE-1				
SEM V	**CHH309**	Application of computers in Chemistry	DSE-1	4-0-0	4
	CHH311	Application of computers in Chemistry- Lab	DSE Lab -1	0-0-4	2
	CHH313	Analytical Methods in chemistry	DSE-1	4-0-0	4
	CHH315	Analytical Methods in chemistry-Lab	DSE Lab -1	0-0-4	2
	Select any one DSE-2				
	CHH317	Industrial Chemicals and Environment	DSE-2	4-0-0	4
	CHH319	Industrial Chemicals and Environment- Lab	DSE Lab-2	0-0-4	2
	CHH321	Novel Inorganic Solids	DSE-2	4-0-0	4
	CHH323	Novel Inorganic Solids- Lab	DSE Lab-2	0-0-4	2
	Select any one DSE-3				
SEM VI	**CHH310**	Polymer chemistry	DSE-3	4-0-0	4
	CHH312	Polymer chemistry- Lab	DSE Lab-3	0-0-4	2
	CHH314	Green Chemistry	DSE-3	4-0-0	4
	CHH316	Green Chemistry- Lab	DSE Lab-3	0-0-4	2
	Select any one DSE-4				
	CHH318	Molecular Modelling and Drug Designing	DSE-4	4-0-0	4
	CHH320	Molecular Modelling and Drug Designing- Lab	DSE Lab-4	0-0-4	2
	CHH322	Inorganic material and Industrial importance	DSE-4	4-0-0	4
	CHH324	Inorganic material and Industrial importance- Lab	DSE Lab-4	0-0-4	2

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

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 Chemical Kinetics (4 + 4)
8. Inorganic Chemistry III: Coordination Chemistry (4 + 4)
9. Organic Chemistry III: Heterocyclic Chemistry (4 + 4)
10. Physical Chemistry IV: Electrochemistry (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)

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

1. Mathematics (5) + Tut (1)
2. Physics (4) + Lab (4)
3.Biotechnology(4) + Lab(4)

Skill Enhancement Courses (Credit: 04 each)-

1. Intellectual Property Rights
2. Pharmaceutical Chemistry

Table 2; Generic Elective Papers (GE) (Minor-Chemistry) for other Departments/Disciplines: (Credit: 06 each)

Semester	Course Code	Course Name	Category	L-T-P	Credits
SEM I	**CHH109**	Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons	Generic Elective -1	4-0-0	4
	CHH111	Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons- Lab	Generic Elective -1 Practical	0-0-4	2
SEM II	**CHH110**	Chemical Energetic, Equilibria and Functional Organic Chemistry	Generic Elective -2	4-0-0	4

	CHH112	Chemical Energetic, Equilibria and Functional Organic Chemistry- Lab	Generic Elective -2 Practical	0-0-4	2
SEM III	**CHH215**	Solutions, Phase Equilibria, Conductance, Electrochemistry, & Functional Group Organic Chemistry	Generic Elective -3	4-0-0	4
	CHH217	Solutions, Phase Equilibria, Conductance, Electrochemistry, & Functional Group Organic Chemistry- Lab	Generic Elective -3 Practical	0-0-4	2
SEM IV	**CHH216**	Organometallics, Bio-inorganic Chemistry, Polynuclear Hydrocarbons & UV, IR Spectra	Generic Elective -4	4-0-0	4
	CHH218	Organometallics, Bio-inorganic Chemistry, Polynuclear Hydrocarbons & UV, IR Spectra- Lab	Generic Elective -4 Practical	0-0-4	2

New course structure will be effective from academic session 2019-20. School/Department will not be bound to run all the courses. Minimum number of students may be fixed to run any elective course.

CORE COURSE (HONOURS IN CHEMISTRY)

Semester I

CHH101: INORGANIC CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Atomic Structure

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and $\psi 2$. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number. **(14 Lectures)**

Unit 2: Periodicity of Elements:

s, p, d, f block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to *s* and *p*-block.

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

(b) Atomic radii (van der Waals)

(c) Ionic and crystal radii.

(d) Covalent radii (octahedral and tetrahedral)

(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.

(f) Electron gain enthalpy, trends of electron gain enthalpy.

(g) Electronegativity, Pauling's/ Mulliken's/ Allred RaCHow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial CHarge, hybridization, group electronegativity. Sanderson's electron density ratio. **(16 Lectures)**

Unit 3: Chemical Bonding I

(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). Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths.

Unit 4: Chemical Bonding II

(i) Covalent Character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

(ii)Ionic Character in covalent compounds: Bond moment and dipole moment. Percentage ionic Character from dipole moment and electronegativity difference.

(iii) *Metallic Bond:* Qualitative idea of valence bond and band theories. Semiconductors and

insulators, defects in solids.

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

Unit 5: Oxidation-Reduction:

Redox equations, Standard Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class. **(4 Lectures)**

Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970
- Atkins, P.W. & Paula, J. *Physical Chemistry*, 10th Ed., Oxford University Press, 2014.
- Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
- Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.

CHH103 : INORGANIC CHEMISTRY LAB- I **60 Lectures**

(A) Titrimetric Analysis

(i) Calibration and use of apparatus

(ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

(i) Estimation of carbonate and hydroxide present together in mixture.

(ii) Estimation of carbonate and bicarbonate present together in a mixture.

(iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

(i) Estimation of Fe(II) and oxalic acid using standardized KMnO4 solution.

(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.

(iii) Estimation of Fe(II) with K2Cr2O7 using internal (diphenylamine, anthranilic acid) and external indicator.

Reference text:

1. Mendham, J., A. I. Vogel's *Quantitative CHemical Analysis 6th Ed.,* Pearson, 2009.

CHH105: PHYSICAL CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Gaseous state I

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.

Unit 2: Gaseous state II

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, *Z*, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour,

virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and Van der Waals constants

(18 Lectures)

Unit 3: Liquid state

Qualitative treatment of the structure of the liquid state; Radial distribution function; 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)**

Unit 4: 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,. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. **(16 Lectures)**

Unit 5: Ionic equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical Chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

(20 Lectures)

Reference Books:

 Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University Press (2014).

 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).

 Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

CHH107 : PHYSICAL CHEMISTRY LAB- I

60 Lectures

1. **Surface tension measurements.**

a. Determine the surface tension by (i) drop number (ii) drop weight method.

b. Study the variation of surface tension of detergent solutions with concentration.

2. Viscosity measurement using Ostwald's viscometer.

a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.

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

3. pH metry

a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid,

sodium acetate and their mixtures.

b. Preparation of buffer solutions of different pH

i. Sodium acetate-acetic acid

ii. Ammonium CHloride-ammonium hydroxide

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

d. Determination of dissociation constant of a weak acid.

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

CHH102: ORGANIC CHEMISTRY- I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1:Basics of Organic Chemistry

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

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

relative strength.

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal Charges; Electrophiles and Nucleophiles; Nucleophlicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes. **(6 Lectures)**

Unit 2: Stereochemistry

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: cis–trans and, syn-anti isomerism 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 resolution. Relative and absolute configuration: D/L and R/S designations.

(18 Lectures)

Unit 3: Chemistry of Aliphatic Hydrocarbons

A. Carbon-Carbon sigma bonds

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

B. Carbon-Carbon pi bonds:

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

Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and Chemical), syn and anti-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and, Diels-Alder reaction;

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

C. Cycloalkanes and Conformational Analysis

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane: Chair, Boat and Twist boat forms; Relative stability with energy diagrams. **(24 Lectures)**

Unit 4: 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.
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

CHH104: ORGANIC CHEMISTRY LAB- I

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 above compounds and 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)

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)

CHH106: PHYSICAL CHEMISTRY- II

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Chemical Thermodynamics

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

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*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermo Chemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of 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)**

Unit 2: 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)**

Unit 3: Chemical Equilibrium:

Criteria of thermodynamic equilibrium, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between

Gibbs free energy of reaction and reaction quotient. reactions. Equilibrium constants and their quantitative dependence on temperature, pressure

and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants *Kp, Kc* and *Kx*. Le CHatelier principle (quantitative treatment) **(8 Lectures)**

Unit 4: 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* 10th Ed., Oxford University Press (2014).
- 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).

CHH108: PHYSICAL CHEMISTRY LAB- II

60 Lectures

Thermo Chemistry

(a) Determination of heat capacity of a calorimeter for different volumes using Change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).

(b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) Calculation of the enthalpy of ionization of ethanoic acid.

(d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) Determination of basicity/proticity of a polyprotic 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 copper sulphate.

(g) Study of the solubility of benzoic acid in water and determination of ΔH.

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).

Semester III

CHH201: INORGANIC CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: General Principles of Metallurgy

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

(6 Lectures)

Unit 2: Acids and Bases

Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB) Application of HSAB principle.

(8 Lectures)

Unit 3: Chemistry of *s* and *p* Block Elements

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements.

Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses.

Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, Phosphorus and CHlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens. **(30 Lectures)**

Unit 4: Noble Gases

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2, XeF_4 and XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF2). Molecular shapes of noble gas compounds (VSEPR theory). **(8 Lectures)**

Unit 5: Inorganic Polymers

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

Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
- 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.
- Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4th Ed., Pearson, 2010.
- Atkin, P. *Shriver & Atkins' Inorganic Chemistry* 5th Ed. Oxford University Press (2010).

CHH203 :INORGANIC CHEMISTRY LAB- II **60 Lectures**

(A) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).

(ii) Estimation of available Chlorine in bleaching powder iodometrically.

(B) Inorganic preparations

(i) Cuprous Chloride, Cu_2Cl_2

(ii) Preparation of Manganese(III) phosphate, $MnPO_4.H_2O$

(iii) Preparation of Aluminium potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.

Reference Books:

Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.

CHH205: ORGANIC CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Chemistry of Halogenated Hydrocarbons:

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – SN_1, SN_2 and SNi mechanisms with stereo chemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; SNAr, Benzyne mechanism.

Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions. **(16 Lectures)**

Unit 2: Alcohols, Phenols, Ethers and Epoxides

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3°

alcohols, Bouvaelt-Blanc Reduction; Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;

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

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$ (**16 Lectures)**

Unit 3: Carbonyl Compounds

Structure, reactivity and preparation;

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

(**14 Lectures)**

Unit 4: Carboxylic Acids and their Derivatives:

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic sustitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Reformatsky reactions, Hofmannbromamide degradation and Curtius rearrangement. **(10 Lectures)**

Unit 5: Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids. **(4 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.

 McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

CHH207:ORGANIC CHEMISTRY LAB- II

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. Oxidation of ethanol/ isopropanol (Iodoform reaction).

iii. Nitration of any one of the following:

a. Acetanilide/nitrobenzene by conventional method

b. Salicylic acid by green approach (using ceric ammonium nitrate).

iv. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.

v. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.

vi. Hydrolysis of amides and esters.

vii. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

viii. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).

ix. Aldol condensation using either conventional or green method.

x. Benzil-Benzilic acid rearrangement.

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, melting point and TLC.

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).

CHH209 : PHYSICAL CHEMISTRY-III (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: 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 solidliquid,liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

Three component systems, water-chloroform-acetic acid system, triangular plots.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst distribution law: its derivation and applications. **(28 Lectures)**

Unit 2: 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. **(18 Lectures)**

Unit 3: Catalysis

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis. **(8 Lectures)**

Unit 4: Surface chemistry

Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state.

(6 Lectures)

Reference Books:

 Peter Atkins & Julio De Paula, *Physical Chemistry* 10th Ed., Oxford University Press (2014).

 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).

CHH211: PHYSICAL CHEMISTRY LAB- III

60 Lectures

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

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

a. simple eutectic and

b. congruently melting systems.III. Distribution of acetic/ benzoic acid between water and Initial rate method: Iodide-persulphate reaction

2. Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

3. Compare the strengths of HCl and H2SO4 by studying kinetics of hydrolysis of methyl acetate.

III. Adsorption

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

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 IV

CHH202: INORGANIC CHEMISTRY-III

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: 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 (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). 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)**

Unit 2: 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 & Bsworth diagrams). Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy) **(18 Lectures)**

Unit 3: Lanthanoids and Actinoids:

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

(6 Lectures)

Unit 4: Bioinorganic Chemistry:

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

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

(10 Lectures)

Reference Books:

 Purcell, K.F & Kotz, J.C. *Inorganic Chemistry* W.B. Saunders Co, 1977.

 Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.

 Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry* Panima Publishing Company 1994.

 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.

CHH204: INORGANIC CHEMISTRY LAB- III

60 Lectures

Gravimetric Analysis:

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).

ii. Estimation of copper as CuSCN

iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

iv. Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

Inorganic Preparations:

i. Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

ii. *Cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)

iii. Tetraamminecarbonatocobalt (III) ion

iv. Potassium tris(oxalate)ferrate(III)

Chromatography of metal ions

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

i. Ni (II) and Co (II)

ii. Fe (III) and Al (III)

Reference Book:

Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.

CHH206: ORGANIC CHEMISTRY-III

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Nitrogen Containing Functional Groups

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

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

Diazonium Salts: Preparation and their synthetic applications. **(18 Lectures)**

Unit 2: Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons. **(8 Lectures)**

Unit 3: 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), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Derivatives of furan: Furfural and furoic acid. **(22 Lectures)**

Unit 4: Alkaloids

Natural occurrence and classification, General structural features, Isolation and their physiological action, Hoffmann's exhaustive methylation, Emde's modification, Structure synthesis and medicinal importance of Nicotine. **(6 Lectures)**

Unit 5: Terpenes

Occurrence, classification, isoprene rule; Elucidation of stucture and synthesis of α-terpineol. **(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.
- McMurry, J.E. *Fundamentals of Organic Chemistry,* 7th Ed. Cengage Learning India Edition, 2013.
- 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,* Prajati Parakashan (2010).

CHH208: ORGANIC CHEMISTRY LAB- III

60 Lectures

1. Detection of extra elements.

2. Functional group test for nitro, amine and amide groups.

3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

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).

CHH210 : PHYSICAL CHEMISTRY-IV

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Conductance

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager

equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

(20 Lectures)

Unit 2: Electrochemistry

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, 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, Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Potentiometric titrations (acid-base, redox, precipitation). **(28 Lectures)**

Unit 3: Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement **(12 Lectures)**

Reference Books:

 Atkins, P.W & Paula, J.D. *Physical Chemistry*, 10th Ed., Oxford University Press (2014).

 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).

CHH212: PHYSICAL CHEMISTRY LAB - IV

60 Lectures

Conductometry

I. Determination of cell constant

II. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

III. Perform the following conductometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

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

iv. Strong acid vs. weak base

Potentiometry

I Perform the following potentiometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. Dibasic acid vs. strong base

iv. Potassium dichromate vs. Mohr's salt

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 V

CHH301: ORGANIC CHEMISTRY-IV

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides; Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine;Structure of polynucleotides. **(9 Lectures)**

Unit 2: Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

α-Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, p*K*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 **(16 Lectures)**

Unit 3: 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 and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition). (8 Lectures)

Unit 4: Lipids

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

(8 Lectures)

Unit 5: 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.

Overview of catabolic pathways of fat and protein.

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

Caloric value of food, standard caloric content of food types. **(7 Lectures)**

Unit 6: 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. & Stryer, L. (2006) *Biochemistr*y. 6th Ed. W.H. Freeman and Co.

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

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

CHH303: ORGANIC CHEMISTRY LAB IV

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.

CHH305: PHYSICAL CHEMISTRY V

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Quantum Chemistry

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

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

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

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 H2.

Comparison of LCAO-MO and VB treatments of H2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. **(24 Lectures)**

Unit 2: Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

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

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

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

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

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

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

simple radicals. **(24 Lectures)**

Unit 3: 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:

- 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).
- Kakkar, R. *Atomic & Molecular Spectroscopy*: *Concepts & Applications*, Cambridge University Press (2015).
- Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).

CHH307:PHYSICAL CHEMISTRY LAB- V

60 Lectures

UV/Visible spectroscopy

I. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λmax 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 K2Cr2O7.

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

Colourimetry

I**.** Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

II. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ 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-phenathroline.

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 HCl(g)

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 VI

CHH302 : INORGANIC CHEMISTRY-IV (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Theoretical Principles in Qualitative Analysis (H_2S Scheme)

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

Unit 2: 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. □-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

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

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene. **(22 Lectures)**

Unit 3: Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes,

Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes.

(18 Lectures)

Unit 4: Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinsons Catalyst)

2. Hydroformylation (Co salts)

3. Wacker′s Process

4. Synthetic gasoline (Fischer Tropsch reaction)

5. Synthesis gas by metal carbonyl complexes **(10 Lectures)**

Reference Books:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall, 1996.
- Cotton, F.A.G.; Wilkinson & 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 Chemistry3rd Ed., John Wiley and Sons, NY, 1994.

- Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements, Elsevier 2nd Ed,*

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. & P. Atkins, *Inorganic Chemistry 2nd Ed.,* Oxford University Press,1994.

 Basolo, F. & Pearson, R. *Mechanisms of Inorganic Reactions: Study of Metal*

Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.

 Purcell, K.F. & Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977

 Miessler, G. L. & Tarr, D.A. *Inorganic Chemistry 4th Ed.,* Pearson, 2010.

 Collman, J. P. *et al. Principles and Applications of Organotransition Metal Chemistry*. Mill Valley, CA: University Science Books, 1987.

 Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*. *j* New

York, NY: John Wiley, 2000.

 Spessard, G. O. & Miessler, G.L. *Organometallic Chemistry*. Upper Saddle River,

NJ: Prentice-Hall, 1996.

CHH304: INORGANIC CHEMISTRY LABL- IV

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:CO_3^{2-}, NO^{2-}, S^{2-}, SO_3^{2-},$S_2O_3^{2-}$, CH_3COO^-, F^-,Cl^-, Br^-, I^-, NO_3^-,

BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH^{4+}, K^+,Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+},Sr^{2+}, Ca^{2+},Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$,

$SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) **or** combination of anions e.g. CO_3^2-and SO_3^{2-}, NO_2^- and NO_3^-,Cl^- and Br^-, Cl^- and I^-, $Br^-$and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible.

i. Measurement of 10 Dq by spectrophotometric method

ii. Verification of spectrochemical series.

iii. Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs

thermodynamic factors.

iv. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.

v. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Reference Books

- Vogel's *Qualitative Inorganic Analysis,* Revised by G. Svehla. Pearson Education, 2002.
- Marr & Rockett *Practical Inorganic Chemistry.* John Wiley & Sons 1972.

CHH306 : ORGANIC CHEMISTRY-V (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: 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)

Unit 2: 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)**

Unit 3: Dyes

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

Synthesis and applications of: Azo dyes – Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet;

Phthalein Dyes – Phenolphthalein and Fluorescein . **(8 Lectures)**

Unit 4: Polymers

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

Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index. Polymerisation reactions -Addition and condensation – Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes; Preparation and applications of plastics – thermosetting (phenol-formaldehyde,Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics – natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and

synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives; Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples. **(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.

 McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

 Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.

 Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry,* Prajati Prakashan (2010).

 Kemp, W. *Organic Spectroscopy,* Palgrave.

 Pavia, D. L. *et al. Introduction to Spectroscopy* 5th Ed. Cengage Learning India Ed. (2015).

CHH308 : ORGANIC CHEMISTRY LAB- V

60 Lectures

1. Extraction of caffeine from tea leaves.

2. Preparation of sodium polyacrylate.

3. Preparation of urea formaldehyde.

4. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.

5. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for e.g. salicylic acid, cinnamic acid, nitrophenols, etc.

6. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).

7. 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).

CHEMISTRY-DSE I-IV (ELECTIVES)

CHH309 : APPLICATIONS OF COMPUTERS IN CHEMISTRY
(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: Basics:

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

Unit 2: Numerical methods:

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

Differential calculus: Numerical differentiation.

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

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

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

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

Reference Books:

- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).

 Venit, S.M. *Programming in BASIC: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).

CHH311: DSE LAB-1- APPLICATIONS OF COMPUTERS IN CHEMISTRY

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, Compressibilty 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 Chemsketch, Arguslab and Accelerys 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).

CHH313: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1 :Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals. **(5 Lectures)**

Unit 2*:* Optical methods of analysis: Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

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

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

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

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

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples. **(25 Lectures)**

Unit 3: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)**

Unit 4: Electro analytical methods: Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values. **(10 Lectures)**

Unit 5: Separation techniques: Solvent extraction: Classification, principle and efficiency of the technique.Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions.Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media. Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods.

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

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

chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis. **(15 Lectures)**

Reference Books:

 Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.

 Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.

 Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.

 Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.

 Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.

 Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.

 Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.

 Ditts, R.V. Analytical Chemistry; Methods of separation, van Nostrand, 1974.

CHH315: DSE LAB-1 -ANALYTICAL METHODS IN CHEMISTRY

60 Lectures

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.

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

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

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

II. Solvent Extractions:

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

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

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

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

5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange:

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

(ii) Separation of metal ions from their binary mixture.

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

III Spectrophotometry

1. Determination of pKa values of indicator using spectrophotometry.

2 Structural characterization of compounds by infrared spectroscopy.

3 Determination of dissolved oxygen in water.

4 Determination of chemical oxygen demand (COD).

5 Determination of Biological oxygen demand (BOD).

6 Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

Reference Books:

 Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.

 Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.

 Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.

 Harris, D.C. *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.

 Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.

 Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Edition.

 Mikes, O. & Chalmes, R.A. *Laboratory Handbook of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.

 Ditts, R.V. *Analytical Chemistry: Methods of separation.* Van Nostrand, New York, 1974.

CHH317: INDUSTRIAL CHEMICALS AND ENVIRONMENT

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: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)**

Unit 2:Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology. **(4 Lectures)**

Unit 3: Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

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

Pollution by SO_2, CO_2, CO, NOx, H_2S and other foul smelling gases. Methods of estimation of CO, NOx, SOx 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)**

Unit 4: 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)**

Unit 5: 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).

CHH319 : DSE LAB -2 - INDUSTRIAL CHEMICALS AND ENVIRONMENT

60 Lectures

1. Determination of dissolved oxygen in water.

2. Determination of Chemical Oxygen Demand (COD)

3. Determination of Biological Oxygen Demand (BOD)

4. Percentage of available chlorine in bleaching powder.

5. Measurement of chloride, sulphate and salinity of water samples by simple titration method ($AgNO_3$ and potassium chromate).

6. Estimation of total alkalinity of water samples (CO_3^{2-}, HCO_3^-) using double titration method.

7. Measurement of dissolved CO_2.

8. Study of some of the common bio-indicators of pollution.

9. Estimation of SPM in air samples.

10. Preparation of borax/ boric acid.

Reference Books:

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

CHH321: NOVEL INORGANIC SOLIDS (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: 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)**

Unit 2: Inorganic solids of technological importance

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals. **(10 Lectures)**

Unit 3: 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, Bio-nano composites. **(10 Lectures)**

Unit 4: 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)**

Unit 5: 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)**

Unit 6: Speciality polymers

Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene and polypyrrole, applications of conducting polymers, Ion-exchange resins and their applications. Ceramic & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications. **(10 Lectures)**

Reference Books:

 Shriver & Atkins. *Inorganic Chemistry*, Peter Alkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)

 Adam, D.M. *Inorganic Solids: An introduction to concepts in solid-state structural chemistry*. John Wiley & Sons, 1974.

 Poole, C.P. & Owens, F.J. *Introduction to Nanotechnology* John Wiley & Sons, 2003.

 Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.

CHH323 :DSE LAB-2- NOVEL INORGANIC SOLIDS

60 Lectures

1. Determination of cation exchange method

2. Determination of total difference of solids.

3. Synthesis of hydrogel by co-precipitation method.

4. Synthesis of silver and gold metal nanoparticles.

Reference Book:

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

CHH310 : POLYMER CHEMISTRY

(Credits: Theory-06, Practicals-02)

Theory: 60 Lectures

Unit 1: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)**

Unit 2: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)**

Unit 3: 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)**

Unit 4 :Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. **(4 Lectures)**

Unit 5: Nature and structure of polymers-Structure Property relationships. **(2 Lectures)**

Unit 6: Determination of molecular weight of polymers (*Mn*, *Mw*, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. **(8 Lectures)**

Unit 7 : Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg). **(8 Lectures)**

Unit 8 : Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of

(8 Lectures)

Unit 9: Properties of Polymers (Physical, thermal, Flow & Mechanical Properties).

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

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

(10 Lectures)

Reference Books:

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

CHH312 : DSE LAB- 3 -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-isobutylonitrile (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. $NaNO_2$ solution

(b) (Poly vinyl proplylidine (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:

 Malcohm 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).

CHH314 : GREEN CHEMISTRY (Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: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)**

Unit 2:Principles of Green Chemistry and Designing a Chemical synthesis

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

 Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.

 Prevention/ minimization of hazardous/ toxic products reducing toxicity. risk = (function) hazard × exposure; waste or pollution prevention hierarchy.

 Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, immobilized solvents

and how to compare greenness of solvents.

 Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.

 Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.

 Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.

 Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) 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)**

Unit 3: Examples of Green Synthesis/ Reactions and some real world cases

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

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

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

4 Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.

5 Designing of Environmentally safe marine antifoulant.

6 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.

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

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

9 Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting **(16 Lectures)**

Unit 4: 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 Lectures)**

Reference Books:

 Ahluwalia, V.K. & Kidwai, M.R. *New Trends in Green Chemistry*, Anamalaya Publishers (2005).

 Anastas, P.T. & Warner, J.K.: *Green Chemistry - Theory and Practical*, Oxford University Press (1998).

 Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).

 Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).

 Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).

 Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition, 2010.

CHH316: DSE LAB-3 - GREEN CHEMISTRY

60 Lectures

1. Safer starting materials

 Preparation and characterization of nanoparticles of gold using tea leaves.

2. Using renewable resources

 Preparation of biodiesel from vegetable/ waste cooking oil.

3. Avoiding waste

Principle of atom economy.

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

 Preparation of propene by two methods can be studied

(I) Triethylamine ion + OH^- → propene + trimethylpropene + water

(II) 1-propanol

H_2SO_4/propene + water

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

4. Use of enzymes as catalysts

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

5. Alternative Green solvents

Extraction of D-limonene from orange peel using liquid CO_2 prepared form dry ice.

Mechanochemical solvent free synthesis of azomethines

6. Alternative sources of energy

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

 Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

Reference Books:

 Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice,* Oxford University Press (1998).

 Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).

 Ryan, M.A. *Introduction to Green Chemistry,* Tinnesand; (Ed), American Chemical Society, Washington DC (2002).

 Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. *Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi*. Bangalore CISBN 978-93-81141-55-7 (2013).

 Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry,* American Chemical Society (2008).

 Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry,* American Chemical Society (2008).

 Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition, 2010.

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

CHH318: MOLECULAR MODELLING & DRUG DESIGN

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1: 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)**

Unit 2: 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)**

Unit 3: 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)**

Unit 4: 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)**

Unit 5: Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design, Drug Discovery – Chemoinformatics – QSAR. **(12 Lectures)**

Reference Books:

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

CHH320: DSE LAB-4 - 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, N_2, 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 ºC, 100 ºC, 108 ºC, 82 ºC, 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 H_2O, H_2S, H_2Se. (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.
- Gupta, S.P. *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.

CHH 322: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1:Silicate Industries

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

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

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements. **(16 Lectures)**

Unit 2: Fertilizers

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate. **(8 Lectures)**

Unit 3: Surface Coatings

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing. **(10 Lectures)**

Unit 4 :Batteries

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell. **(6 Lectures)**

Unit 5 : Alloys

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels. **(10 Lectures)**

Unit 6: Catalysis

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

Phase transfer catalysts, application of zeolites as catalysts. **(6 Lectures)**

Unit 7: Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants. **(4 Lectures)**

Reference Books:

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

 R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.

 W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics,* Wiley Publishers, New Delhi.

 J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.

 P. C. Jain, M. Jain: *Engineering Chemistry,* Dhanpat Rai & Sons, Delhi.

 R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry,* Vikas Publications, New Delhi.

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

CHH 324: LAB-4- INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

60 Lectures

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

Reference Books:

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

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

Skill Enhancement Course (Credit: 04 each)

CHH213: INTELLECTUAL PROPERTY RIGHTS (IPR)

(Credits: Theory-04)

Unit 1: Introduction to Intellectual Property:

Historical Perspective, Different Types of IP, Importance of protecting IP.

Unit 2: Copyrights

Introduction, How to obtain, Differences from Patents.

Unit 3: Trade Marks

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

Unit 4: 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.

Unit 5: Geographical Indications

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

Unit 6: Industrial Designs

Definition, How to obtain, features, International design registration.

Unit 7: Layout design of integrated circuits

Circuit Boards, Integrated Chips, Importance for electronic industry.

Unit 8: Trade Secrets

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

Unit 9: Different International agreements

(a) Word 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

Unit 10: 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:

- Acharya, N.K. *Textbook on intellectual property rights*, Asia Law House (2001).
- Guru, M. & Rao, M.B. *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).
- Ganguli, P. *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill (2001).
- Miller, A.R. & Davis, M.H. *Intellectual Property: Patents, Trademarks and Copyright in a Nutshell*, West Group Publishers (2000).
- Watal, J. *Intellectual property rights in the WTO and developing countries*, Oxford University Press, New Delhi.

CHH214: PHARMACEUTICAL CHEMISTRY

(Credits: Theory-04)

Unit 1: 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, lbuprofen); 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).

Unit 2: 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 B_2, Vitamin B_{12} and Vitamin C.

Practicals

1. Preparation of Aspirin and its analysis.

2. Preparation of magnesium bisilicate (Antacid).

Reference Books:

- Patrick, G. L. *Introduction to Medicinal Chemistry, Oxford University* Press, UK, 2013.
- Singh, H. & Kapoor, V.K. *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan, Pitampura, New Delhi, 2012.
- Foye, W.O., Lemke, T.L. & William, D.A.: *Principles of Medicinal Chemistry*, 4th ed., B.I. Waverly Pvt. Ltd. New Delhi.

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

CHH109: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

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

Unit 1: Atomic Structure: *Review of: Bohr's theory and its limitations, dual behaviour of Matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.*What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2, Schrödinger equation for hydrogen atom. Radial and angular parts of the hydogenic wavefunctions (atomic orbitals) and their variations for 1*s*, 2*s*, 2*p*, 3*s*, 3*p* and 3*d* 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 1*s* and 2*s* atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers *ml* and *ms*. Shapes of *s*, *p* and *d* atomic orbitals, nodal planes. Discovery of spin, spin quantum number (*s*) and magnetic spin quantum number (*ms*).

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)**

Unit 2: Chemical Bonding and Molecular Structure

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability.

Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

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

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

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for *s-s*, *s-p* and *p-p* combinations of atomic orbitals, nonbonding combination (including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and NO+. Comparison of VB and MO approaches. **(16 Lectures)**

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

Unit 1: Fundamentals of Organic Chemistry

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

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles.

Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule. **(8 Lectures)**

Unit 2 : 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)**

Unit 3: Aliphatic Hydrocarbons

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

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

Alkenes: (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). *Reactions:* cis-addition (alk. $KMnO_4$) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. *Reactions:* formation of metal acetylides, addition of bromine and alkaline $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$. **(12 Lectures)**

Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.
- Graham Solomon, T.W., Fryhle, C.B. & Dnyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

 Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).

 Eliel, E.L. *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2000.

 Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.

 Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.

 Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

CHH111:GE LAB 1- 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 $K_2Cr_2O_7$ using internal indicator.

5. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)

2. Separation of mixtures by Chromatography: Measure the R*f* value in each case (combination of two compounds to be given)

(a) Identify and separate the components of a given mixture of two 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:

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

CHH110: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

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

Unit 1: 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)**

Unit 2: Chemical Equilibrium

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG^{o}, Le Chatelier's principle. Relationships between *Kp, Kc* and *Kx* for reactions involving ideal gases. **(8 Lectures)**

Unit 3: Ionic Equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. **(12 Lectures)**

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

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

Unit 1: Aromatic hydrocarbons

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

Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene). **(8 Lectures)**

Unit 2: Alkyl and Aryl Halides

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

Preparation: from alkenes *and* alcohols.

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

Unit 3: Aryl Halides *Preparation:* (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions.

Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides. **(8 Lectures)**

Unit 4: Alcohols, Phenols and Ethers (Upto 5 Carbons)

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

Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation *Diols:* (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Unit 5: Phenols: (Phenol case) *Preparation:* Cumene hydroperoxide method, from diazonium salts.

Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer81 Tiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten – Baumann Reaction.

Unit 6: Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

Unit 7: Aldehydes and ketones (aliphatic and aromatic): (Formaldehye, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and from nitriles.

Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Pondorff Verley reduction. **(14 Lectures)**

Reference Books:

- Graham Solomon, T.W., Fryhle, C.B. & Dnyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.

 Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).

 Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.

 Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.

 Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

 Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).

 Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).

 Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).

 Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).

 Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

CHH112: GE LAB 2 - CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY-I

60 Lectures

Section A: Physical Chemistry

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes.

2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

3. Determination of enthalpy of ionization of acetic acid.

4. Determination of integral enthalpy of solution of salts (KNO_3, NH_4Cl).

5. Determination of enthalpy of hydration of copper sulphate.

6. Study of the solubility of benzoic acid in water and determination of ΔH.

Ionic equilibria

pH measurements

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.

a) Preparation of buffer solutions:

(i) Sodium acetate-acetic acid

(ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.

2. Criteria of Purity: Determination of melting and boiling points.

3. Preparations: Mechanism of various reactions involved to be discussed.

Recrystallisation, determination of melting point and calculation of quantitative yields to be done.

(a) Bromination of Phenol/Aniline

(b) Benzoylation of amines/phenols

(c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone

Reference Books

 Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.

 Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

 Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R.Chand & Co.: New Delhi (2011).

CHH215 : CHEMISTRY OF MAIN GROUP ELEMENTS, THEORIES OF ACIDS AND BASES

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Unit 1 :Acids and Bases

Brönsted–Lowry concept, conjugate acids and bases, relative strengths of acids and bases, effects of substituent and solvent, differentiating and levelling solvents. Lewis acid-base concept, classification of Lewis acids and bases, Lux-Flood concept and solvent system concept. Hard and soft acids and bases (HSAB concept), applications of HSAB process. **(10 Lectures)**

Unit 2: 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 agents.Hydrometallurgy with reference to cyanide process for gold and silver. Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn, Au): electrolytic refining, zone refining, van Arkel-de Boer process, Parting Process, Mond's process and Kroll Process. **(8 Lectures)**

Unit 3: s- and p-Block Elements

Periodicity in *s*- and *p*-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electron gain enthalpy, electronegativity (Pauling scale). General characteristics of *s*-block metals like density, melting and boiling points, flame colour and reducing nature. Oxidation states of *s*- and *p*-block elements, inert-pair effect, diagonal relationships and anomalous behaviour of first member of each group. Allotropy in C, P and S.Complex forming tendency of *s* block elements and a preliminary idea of crown ethers and cryptates, structures of basic beryllium acetate, salicylaldehyde/ acetylacetonato complexes of Group 1 metals.

Solutions of alkali metals in liquid ammonia and their properties.

Common features, such as ease of formation, solubility and stability of oxides, peroxides, superoxides, sulphates and carbonates of *s*-block metals. **(14 Lectures)**

Structure, bonding and properties (acidic/ basic nature, oxidizing/ reducing nature and hydrolysis of the following compounds and their applications in industrial and environmental chemistry wherever applicable:

Diborane and concept of multicentre bonding, hydrides of Groups 13 (EH3), 14, 15, 16 and 17. Oxides of N and P, Oxoacids of P, S and Cl. Halides and oxohalides of P and S (PCl_3, PCl_5, $SOCl_2$ and SO_2Cl_2) Interhalogen compounds.

A brief idea of pseudohalides **(14 Lectures)**

Unit 4: Noble gases

Rationalization of inertness of noble gases, clathrates, preparation and properties of XeF_2, XeF_4 and XeF_6 ,bonding in these compounds using VBT and shapes of noble gas compounds using VSEPR Theory **(5 Lectures)**

Unit 5: Inorganic Polymers

Types of inorganic polymers and comparison with organic polymers, structural features, classification and important applications of silicates. Synthesis, structural features and applications of silicones. Borazines and cyclophosphazenes – preparation, properties and reactions. Bonding in $(NPCl_2)_3$**.** **(9 Lectures)**

Recommended texts:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry,* 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry,* John Wiley & Sons.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann.1997.

Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.

Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4th Ed., Pearson, 2010.

Atkin, P. *Shriver & Atkins' Inorganic Chemistry* 5th Ed. Oxford University Press (2010).

CHH217 : GE LAB- CHEMISTRY OF MAIN GROUP ELEMENTS, THEORIES OF ACIDS AND BASES

60 Periods

1.Iodometric estimation of potassium dichromate and copper sulphate

2.Iodimetric estimation of antimony in tartaremetic

3.Estimation of amount of available chlorine in bleaching powder and household bleaches

4.Estimation of iodine in iodized salts.

5.Iodimetric estimation of ascorbic acid in fruit juices.

6.Estimation of dissolved oxygen in water samples.

7.Gravimetric estimation of sulphate as barium sulphate.

8.Gravimetric estimation of aluminium as oximato complex

9.Preparation of the following: potash alum, chrome alum, tetraamminecopper(II) sulphate monohydrate, potassium trioxalatoferrate(III) (any two, including one double salt and one complex).

Recommended Texts:

Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.

Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.

CHH216: ORGANOMETALLICS, BIOINORGANIC CHEMISTRY, POLYNUCLEAR HYDROCARBONS AND UV, IR SPECTROSCOPY

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Section A: Inorganic Chemistry-3 **(30 Lectures)**

Unit 1: Chemistry of 3d metals

Oxidation states displayed by Cr, Fe, Co, Ni and Co.

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

Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, sodium nitroprusside, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$. **(6 Lectures)**

Unit 2: Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3*d* metals. p-acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). **(12 Lectures)**

Unit 3: Bio-Inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na^+, K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Role of Ca^{2+} in blood clotting, stabilization of protein structures and structural role (bones). **(12 Lectures)**

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

Unit 4: Polynuclear and heteronuclear aromatic compounds:

Properties of the following compounds with reference to electrophilic and nucleophilic

substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

(6 Lectures)

Unit 5: 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)**

Unit 6: Application of Spectroscopy to Simple Organic Molecules

Application of visible, ultraviolet and infrared spectroscopy in organic molecules. Electromagnetic radiation, electronic transitions, λ_{max} & ε_{max}, chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λmax of conjugated dienes and α,β – unsaturated compounds. Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions). **(18 Lectures)**

Reference Books:

- James E. Huheey, Ellen Keiter & Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
- G.L. Miessler & Donald A. Tarr: *Inorganic Chemistry*, Pearson Publication.
- J.D. Lee: *A New Concise Inorganic Chemistry*, E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley & Sons.
- I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S.
- John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds*, Prentice Hall.

 R.M. Silverstein, G.C. Bassler & T.C. Morrill*: Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.

 R.T. Morrison & R.N. Boyd: *Organic Chemistry*, Prentice Hall.

 Peter Sykes: *A Guide Book to Mechanism* in *Organic Chemistry*, Orient Longman.

 Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.

CHH218: GE LAB-4 -ORGANOMETALLICS, BIOINORGANIC CHEMISTRY, POLYNUCLEAR HYDROCARBONS AND UV, IR SPECTROSCOPY

60 Lectures

Section A: Inorganic Chemistry

1. Separation of mixtures by chromatography: Measure the *Rf* value in each case.

(Combination of two ions to be given)

Paper chromatographic separation of Fe^{3+}, $A1^{3+}$ and Cr^{3+}

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:

a. tetraamminecarbonatocobalt (III) nitrate

b. tetraamminecopper (II) sulphate

c. potassium trioxalatoferrate (III) trihydrate

Compare the conductance of the complexes with that of M/1000 solution of NaCl, $MgCl_2$ and $LiCl_3$.

Section B: Organic Chemistry

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

Reference Books:

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