# CURRICULUM AND CREDIT FRAMEWORK FOR UNDERGRADUATE PROGRAMMES

# **CORE COURSES IN CHEMISTRY**



2025

# COURSE STRUCTURE

# CURRICULUM AND CREDIT FRAMEWORK FOR UNDERGRADUATE PROGRAMMES

C .						DUATETRUGRAM		7D / 1
Semester	Discipline Specific Courses-Core	Minor	Interdisciplinary courses	Ability Enhancement Course (languages)	Skill Enhancement Course /Internship	Dissertation/Project	Common value-added courses	Total Credits
Ĭ	C1:4 C2:4	Min1:4	Environmental Science/CP/ Swayam (3 Credit)	ENG-1 (2 Credit)	SEC: 3 Credit (Common pool)/ Swayam			20
11	C3:4 C4:3	Min2:4	Common Pool/Swayam (3 Credit)	MIL-1/Hindi- 1/Alt Eng-1 (2 Credit)			Soft Skill/NCC/CP/ Swayam (3 Credit)	20
						icate in the relevant Disc	ipline/Subject pro	ovided they
			sed vocational courses			ship/ Apprenticeship	l	
III	C5:4 C6:4	Min3:4	Understanding Heritage/Common Pool/Swayam (3 Credit)	ENG-2 (2 Credit)	SEC: 3 Credit (common pool)/ Swayam			20
IV	C7:4 C8:4	Min4:4		MIL-2/Hindi- 2/Alt Eng-2 (2 Credit)	SEC: 3 Credit (common pool)/ Swayam		Common Pool/NSS/ Swayam (3 Credit)	20
			mme after securing 80 based vocational cours			in the relevant Discipline/S	Subject provided	they secure
V	C09:4 C10:4 C11:4	Min5:4			Internship: 2	,	Work Ethics/CP (2 Credit)	20
VI	C12:4 C13:4 C14:4 C15:4	Min6:4						20
Total	60 Credit	24 Credit	9 Credit	8 Credit	11 Credit		8 Credit	120
	Students who v	want to unde	rtake 3-year UG progr	amme will be awa	arded UG Degree in	the relevant Discipline/Sul	bject upon securin	ng 120
VII	C16:4 C17:4 C18:4 C19:4(Research Methodology)	Min7:4				Research Dissertation will start		20
VIII	C20:4 C21:4** C22:4** C23:4**	Min8:4				C24: Research Project / Dissertation **		20
Total	80 Credit	32 Credit	9 Credit	8 Credit	11 Credit	12 Credit	8 Credit	160

# Major Courses (Core papers):

Paper Code	Course Code	Title of the paper	Total Credit							
FIRST SEMESTER										
C-1	CHEM.C-1 (T)	Inorganic Chemistry I: Atomic Structure &	4							
		Chemical Bonding (3 Credits)								
	CHELL C 4 (P)									
G 2	CHEM.C-1 (P)	Inorganic Chemistry I Lab (1 Credit)	4							
C-2	CHEM.C-2 (T)	Physical Chemistry I: States of Matter & Ionic Equilibrium (3 Credits)	4							
		Tome Equinorium (5 Credits)								
	CHEM.C-2 (P)	Physical Chemistry I Lab (1 Credit)								
SECOND SEMESTER										
C-3	CHEM.C-3 (T) Organic Chemistry I: Basics and		4							
		Hydrocarbons (3 Credits)								
	CHEM.C-3 (P)	Organic Chemistry I Lab (1 Credit)								
C-4	CHEM.C-4 (T)	Physical Chemistry II: Chemical	4							
		Thermodynamics and its Applications (3								
		Credits)								
	CHEM.C-4 (P)	Physical Chemistry II Lab (1 Credit)								
		RD SEMESTER								
C-5	CHEM.C-5 (T)	Inorganic Chemistry II: s- and p-block	4							
		Elements (3 Credits)								
	CHEM.C-5 (P)	Inorganic Chemistry II Lab (1 Credit)								
C-6	CHEM.C-6 (T)	Organic Chemistry II: Oxygen Containing	4							
		Functional Groups (3 Credits)								
	CHEM C ( (D)									
	CHEM.C-6 (P):	Organic Chemistry II Lab (1 Credit) JRTH SEMESTER								
C-7	CHEM.C-7 (T)	Physical Chemistry III: Phase Equilibria and	4							
		Chemical Kinetics (3 Credits)	•							
		, , ,								
~ 0	CHEM.C-7 (P)	Physical Chemistry III Lab (1 Credit)								
C-8	<b>CHEM.C-8 (T)</b>	Inorganic Chemistry III: Coordination Chemistry (3 Credits)	4							
		Chemistry (5 Cledits)								
	CHEM.C-8 (P)	Inorganic Chemistry III Lab (1 Credit)								
FIFTH SEMESTER										
C-9	CHEM.C-9 (T)	Organic Chemistry III: Heterocyclic	4							
		Chemistry (3 Credits)								
	CHEM.C-9 (P)	Organic Chemistry III Lab (1 Credit)								
C-10	CHEM.C-10 (T)	Physical Chemistry IV: Electrochemistry	4							
		(3 Credits)								

	CHEM.C-10 (P)	Physical Chemistry IV Lab (1 Credit)	
C-11	CHEM.C-11 (T)	Organic Chemistry IV: Biomolecules	4
		(3 Credits)	
	CHEM.C-11 (P)	Organic Chemistry IV Lab (1 Credit)	
		XTH SEMESTER	
C-12	CHEM.C-12 (T)	Physical Chemistry V: Quantum Chemistry I	4
0.12		&Spectroscopy (3 Credits)	
	CHEM.C-12 (P)	Physical Chemistry V Lab (1 Credit)	
C-13	CHEM.C-13 (T)	Inorganic Chemistry IV: Organometallic	4
		Chemistry (3 Credits)	
	CHEM.C-13 (P)	Inorganic Chemistry IV Lab (1 Credit)	
C-14	CHEM.C-14 (T)	Organic Chemistry V: Spectroscopy	4
		(3 Credits)	
	CHEM C 14 (D)	One and Characters V. Lab (1 Cas 4.4)	
C-15	CHEM.C-14 (P) CHEM.C-15 (T)	Organic Chemistry V Lab (1 Credit)  Green Chemistry (3 Credits)	4
C-13	CHEWI.C-13 (1)	Green Chemistry (5 Credits)	4
	CHEM.C-15 (P)	Green Chemistry Lab (1 Credit)	
	SE	EVENTH SEMESTER	
C-16	CHEM.C-16 (T)	Inorganic Chemistry V: Fundamentals of	4
0.17	CHEM C 15 (E)	Inorganic Chemistry	4
C-17	CHEM.C-17 (T)	Organic Chemistry VI: Stereochemistry & Organic Transformation Reactions	4
		Organic Transformation Reactions	
C-18	CHEM.C-18 (T)	Physical Chemistry VI: Thermodynamics and	4
		Chemical Dynamics	
C-19	CHEM.C-19 (T)	Research Methodology	4
		EIGHT SEMESTER	
C. 20	CHEM C 20 (D)		4
C-20	CHEM.C-20 (P)	Advanced Laboratory Course in Chemistry	4
C-21	CHEM.C-21 (T)	Inorganic Chemistry VI: Chemistry of The	4
		Elements	
C-22	CHEM.C-22 (T)	Organic Chemistry VII: Synthesis & Reactions	4
C-23	CHEM.C-23 (T)	of Heterocyclic Compounds Physical Chemistry VII: Quantum Mechanics	4
C-23	CITEMI.C-23 (1)	and Statistical Thermodynamics	[
		, and the second	
C-24	CHEM.C-24	Research Project **	12

Each semester contains a minor course of 4 credits
 Students Opting for Honors with research may select research project\*\* instead of C-21, C-22 and C-23

# CHEM.C-1 (T): INORGANIC CHEMISTRY I: ATOMIC STRUCTURE & CHEMICAL BONDING

Total Marks: 100 (Credits: 03)

#### UNIT - I

#### **UNIT – I: Atomic Structure**

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of  $\psi$  and  $\psi^2$ . Quantum numbers and their significance. Normalized and orthogonal wave functions. Shapes of s, p, d orbitals. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

# **UNIT - II: 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) Covalent radii (octahedral and tetrahedral)
- (d) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy.
- (e) Electron gain enthalpy, trends of electron gain enthalpy.
- (f) Electronegativity, Variation of electronegativity with bond order, partial charge, hybridization

## **UNIT - III: Chemical Bonding**

- (i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and itslimitations. Born-Haber cycle and its application, Solvation energy.
- (ii) Covalent bond: Lewis structure, Valence Bond theory (Heitler-London approach). Equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic  $N_2$ ,  $O_2$ ,  $C_2$ ,  $B_2$ ,  $F_2$ , CO, NO, and their ions. Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding ( $\sigma$  and  $\pi$  bond approach) and bond lengths. Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.
- (iii) 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).

# **UNIT - IV: Oxidation-Reduction**

Redox equations and its balancing, Standard Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class.

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

## CHEM.C-1 (P): INORGANIC CHEMISTRY-I Lab

Total Marks: 50 (Credits: 01)

# (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 KMnO<sub>4</sub> solution.
- (ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
- (iii) Estimation of Fe (II) with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> using internal (diphenylamine, anthranilic acid) and external indicator.

### Reference text:

1. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6<sup>th</sup> Ed., Pearson, 2009.

#### CHEM.C-2 (T): PHYSICAL CHEMISTRY I: STATES OF MATTER & IONIC EQUILIBRIUM

Total Marks: 100 (Credits: 03)

#### **UNIT – I: Gaseous state**

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

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

#### UNIT – II: Liquid state

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapour pressure (Determination by Static method), Surface tension (Determination by Drop number method) and Coefficient of viscosity, (Determination by Ostwald's method). 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.

#### **UNIT - III: Solid state**

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X -ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Defects in crystals. Glasses and liquid Crystals.

# UNIT – IV: 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; 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. Theory of acid—base indicators.

- 1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10<sup>th</sup> Ed., Oxford University Press(2014).
- 2. Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- 3. Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed. Narosa (2004).
- 4. Mortimer, R. G. *Physical Chemistry* 3<sup>rd</sup> Ed. Elsevier: NOIDA, UP (2009).
- 5. Engel, T. & Reid, P. *Physical Chemistry* 3<sup>rd</sup> Ed. Pearson (2013).

# CHEM.C-2 (P): PHYSICAL CHEMISTRY-I Lab

Total Marks: 50 (Credits: 01)

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

## 3. Indexing of a given powder diffraction pattern of a cubic crystalline system.

# 4. 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.

- 1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: NewDelhi (2011).
- 2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- 3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3<sup>rd</sup> Ed.; W. H. Freeman & Co.: New York (2003)

### CHEM.C-3 (T): ORGANIC CHEMISTRY I: BASICS AND HYDROCARBONS

Total Marks: 100 (Credits: 03)

### UNIT - I: Basics of Organic Chemistry

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules. *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; Nucleophileity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals.

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

## **UNIT – II: 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.

# **UNIT - III: 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), hydroboration- oxidation, ozonolysis, reduction (catalytic and chemical), 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,

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.

## **UNIT - IV: Aromatic Hydrocarbons**

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and 5, 6-membered 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.

- 1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
- 2. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd.(Pearson

Education).

- 3. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 4. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London,1994.
- 5. Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
- 6. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning IndiaEdition, 2013.

Total Marks: 50 (Credits: 01)

- 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 the 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)

- 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*, 5<sup>th</sup> Ed., Pearson (2012)

# CHEM.C-4 (T): PHYSICAL CHEMISTRY II: CHEMICAL THERMODYNAMICS AND ITS APPLICATIONS

Total Marks: 100 (Credits: 03)

# **UNIT - I: 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 ideal gases under isothermal and adiabatic conditions.

Thermochemistry: 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) 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 the third law, concept of residual entropy, calculation of absolute entropy of molecules from heat capacity data.

Free Energy Functions: Gibbs and Helmholtz energy; variation of G, A with T, V, P; Free energy change and spontaneity. Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

### **UNIT - II: Systems of Variable Composition**

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures.

# **UNIT - III: Chemical Equilibrium**

Types of Chemical equilibrium, Criteria of thermodynamic equilibrium, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of the relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. The thermodynamic derivation of relations between the various equilibrium constants Kp, Kc and Kx. Le Chatelier's principle (quantitative treatment).

#### **UNIT - IV: 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 freezing point, (iv) osmotic pressure and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

- 1. Peter, A. & Paula, J. de. *Physical Chemistry* 10<sup>th</sup> Ed., Oxford University Press (2014).
- 2. Castellan, G. W. Physical Chemistry 4<sup>th</sup> Ed., Narosa (2004).
- 3. Engel, T. & Reid, P. Physical Chemistry 3<sup>rd</sup> Ed., Prentice-Hall (2012).
- 4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
- 5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- 6. Levine, I.N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2010).
- 7. Metz, C.R. 2000. solved problems in chemistry, Schaum Series (2006).

# CHEM.C-4 (P): PHYSICAL CHEMISTRY- II Lab

Total Marks: 50 (Credits: 01)

#### **Thermochemistry**

- (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 temperature 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 the enthalpy of hydration of copper sulphate.
- (g) Study of the solubility of benzoic acid in water and determination of  $\Delta H$ .

Any other experiment carried out in the class.

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

### CHEM.C-5 (T): INORGANIC CHEMISTRY II: S- AND P-BLOCK ELEMENTS

Total Marks: 100 (Credits: 03)

#### UNIT - I: Acids and Bases

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

# UNIT – II: Chemistry of s and p Block Elements

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of the first member of each group. Allotropy and catenation.

Hydrides and their classification: ionic, covalent and interstitial. Basic beryllium acetates and nitrates. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses: Boric acid and borates, boron nitrides, borohydrides (diborane), Oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, pseudo-halogens and basic properties of halogens.

#### **UNIT - III: Noble Gases**

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation, properties and structures of XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub>; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF<sub>2</sub>). Molecular shapes of noble gas compounds XeO<sub>3</sub>, XeOF<sub>2</sub>, XeOF<sub>4</sub> (VSEPR theory).

### **UNIT – IV: Inorganic Polymers**

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones. Borazines, silicates and phosphazenes.

- 1. Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- 2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry3<sup>rd</sup> Ed., John Wiley Sons, N.Y. 1994.
- 3. Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
- 4. Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
- 5. Rodger, G.E. *Inorganic and Solid-State Chemistry*, Cengage Learning India Edition, 2002.
- 6. Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4<sup>th</sup> Ed., Pearson, 2010.
- 7. Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).

# CHEM.C-5 (P): INORGANIC CHEMISTRY-II Lab

Total Marks: 50 (Credits: 01)

# (A) Iodo / Iodimetric Titrations

- (i) Estimation of Cu (II) and K2Cr2O7 using sodium thiosulphate solution (Iodimetrically).
- (ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
- (iii) Estimation of available chlorine in bleaching powder iodometrically.

# (B) Inorganic preparations

- (i) Cuprous Chloride, Cu2Cl2
- (ii) Preparation of Manganese (III) phosphate, MnPO4.H2O
- (iii) Preparation of Aluminium potassium sulphate KAl(SO4)<sub>2</sub>.12H2O (Potash alum) or Chrome alum.
- (iv) Hexaammine Ni (II) Chloride
- (v) Potassium trioxalato chromate (III)
- (vi) Ammonium ferric sulphate
- (vii) Potassium chloro chromate

#### **Reference Books:**

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

# CHEM.C-6 (T): ORGANIC CHEMISTRY II: OXYGEN-CONTAINING FUNCTIONAL GROUPS

Total Marks: 100 (Credits: 03)

## **UNIT - I: Chemistry of Halogenated Hydrocarbons**

Alkyl halides: Methods of preparation, nucleophilic substitution reactions  $-SN^1$ ,  $SN^2$  and  $SN^i$  mechanisms with stereochemical 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. Organometallic compounds of Mg and Li – Use in the synthesis of organic compounds.

# UNIT - II: Alcohols, Phenols, Ethers and Epoxides

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

Phenols: Preparation and properties; Acidity and factors affecting 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 alcohol, ammonia derivatives and LiAlH<sub>4</sub>

#### **UNIT – III: Carbonyl Compounds**

Structure, reactivity and preparation of aldehydes and ketones.

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, Oxidation and reductions (Clemmensen, Wolff-Kishner, LiAlH4, NaBH<sub>4</sub>)

Addition reactions of unsaturated carbonyl compounds: Michael addition.

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

### UNIT - IV: Carboxylic Acids and their Derivatives

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

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

- 1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 3. Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- 4. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

# CHEM.C-6 (P): ORGANIC CHEMISTRY-II Lab

Total Marks: 50 (Credits: 01)

- 1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid groups.
- 2. Organic preparations:
- i. Acetylation of one of the following compounds: amines (aniline, o-, m-, p- toluidines and o-,m-, p-anisidine) and phenols ( $\beta$ -naphthol, vanillin, salicylic acid) by any one method:
- a. Using conventional methods.
- b. Using the green approach
- ii. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p- anisidine) and one of the following phenols ( $\beta$ -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction.
- iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
- iv. Bromination of any one of the following:
- a. Acetanilide by conventional methods
- b. Acetanilide using green approach (Bromate-bromide method)
- v. Nitration of any one of the following:
- a. Acetanilide/nitrobenzene by conventional method
- b. Salicylic acid by the green approach (using ceric ammonium nitrate).
- vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
- vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
- viii. Hydrolysis of amides and esters.
- ix. Semicarbazone of any one of the following compounds: acetone, ethyl methylketone, cyclohexanone, benzaldehyde.
- x. S-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
- xi. Aldol condensation using either conventional or green methods.
- xii. Benzil-Benzilic acid rearrangement.

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

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

### CHEM.C-7 (T): PHYSICAL CHEMISTRY III: PHASE EQUILIBRIA AND CHEMICAL KINETICS

Total Marks: 100 (Credits: 03)

#### UNIT - I: Phase Equilibria

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule, Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one-component systems (Water and Sulphur).

Phase diagrams for systems of solid-liquid equilibria involving eutectic (Silver Lead system), congruent (Ferric Chloride-Water system) and incongruent (Sodium-Potassium system) melting points.

#### **UNIT – II: Chemical Kinetics**

Order and molecularity 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.

## **UNIT -III: Catalysis**

Types of catalysts, 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.

#### **UNIT – IV: Surface chemistry**

Colloids and their classification, Physical adsorption, chemisorption, adsorption isotherms (the Freundlich and Langmuir isotherms). Nature of adsorbed state.

- 1. Peter Atkins & Julio De Paula, *Physical Chemistry* 10<sup>th</sup> Ed., Oxford University Press (2014).
- 2. Castellan, G. W. *Physical Chemistry*, 4th Ed., Narosa (2004).
- 3. McQuarrie, D. A. & Simon, J. D., *Molecular Thermodynamics*, Viva Books Pvt. Ltd.: New Delhi (2004).
- 4. Engel, T. & Reid, P. Physical Chemistry 3<sup>rd</sup> Ed., Prentice-Hall (2012).
- 5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- 6. Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- 7. Ball, D. W. Physical Chemistry Cengage India (2012).
- 8. Mortimer, R. G. *Physical Chemistry 3<sup>rd</sup> Ed.*, Elsevier: NOIDA, UP (2009).
- 9. Levine, I. N. Physical Chemistry 6<sup>th</sup> Ed., Tata McGraw-Hill (2011).
- 10. Metz, C. R. Physical Chemistry 2<sup>nd</sup> Ed., Tata McGraw-Hill (2009).

Total Marks: 50 (Credits: 03)

- I. Determination of critical solution temperature and composition of the phenol-water system, and to study the effect of impurities on it.
- II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
- a. simple eutectic and
- b. congruently melting systems.
- III. Distribution of acetic/ benzoic acid between water and cyclohexane.
- IV. Study the equilibrium of at least one of the following reactions by the distribution method:
- (i)  $I_2(aq) + I \rightarrow I_3(aq)^{2+}$
- (ii)  $Cu^{2+}(aq) + nNH \rightarrow Cu(NH)_{3n}$
- V. Study the kinetics of the following reactions.
- 1. Initial rate method: Iodide-persulphate reaction
- 2. Integrated rate method:
- a. Acid hydrolysis of methyl acetate with hydrochloric acid.
- b. Saponification of ethyl acetate.
- 3. Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying the kinetics of hydrolysis of methylacetate.
- VI. Adsorption
- I. Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

- 1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- 2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- 3. Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3<sup>rd</sup> Ed.; W. H. Freeman & Co.: New York (2003).

# CHEM.C-8 (T): INORGANIC CHEMISTRY III: COORDINATION CHEMISTRY

Total Marks: 100 (Credits: 03)

#### UNIT - I

# **Coordination Chemistry**

Werner's theory, valence bond theory (inner and outer orbital complexes). Crystal field theory, measurement of 10 Dq ( $\Delta_o$ ), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq ( $\Delta_o$ ,  $\Delta_t$ ). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry.

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

# UNIT - II

#### **Transition Elements**

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, and ability to form complexes.

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)

#### UNIT -III

#### Lanthanoids and Actinoids

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

#### UNIT - IV

## **Bioinorganic Chemistry**

Metal ions present in biological systems, classification of elements according to their action in biological system. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals.

Toxicity of metal ions (Hg, Pb, Cd and As), Use of chelating agents in medicine. Iron and its application in bio-systems, Haemoglobin; Storage and transfer of iron.

- Purcell, K. F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- 2. Huheey, J.E., *Inorganic Chemistry*, Prentice Hall, 1993.
- 3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Pub. Co 1994.
- 4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
- 5. Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, 1967.
- 6. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.

## CHEM.C-8 (P): INORGANIC CHEMISTRY-III Lab

Total Marks: 50 (Credits: 01)

## **Gravimetric Analysis:**

- i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
- ii. Estimation of copper as CuSCN
- iii. Estimation of iron as Fe<sub>2</sub>O<sub>3</sub> by precipitating iron as Fe(OH)<sub>3</sub>.
- 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<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>O
- ii. Cis and trans K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>. (H<sub>2</sub>O)<sub>2</sub>] 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 the following metal ions:

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

### **Reference Book:**

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6<sup>th</sup> Ed., Pearson, 2009.

#### CHEM.C-9 (T): ORGANIC CHEMISTRY-III: HETEROCYCLIC CHEMISTRY

Total Marks: 100 (Credits: 01)

#### **UNIT - I: Nitrogen Containing Functional Groups**

Preparation and important reactions of nitro 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.

# **UNIT - II: Polynuclear Hydrocarbons**

Introduction to Polynuclear Hydrocarbons. Reactions of naphthalene, phenanthrene and anthracene. Structure, Preparation and important derivatives of naphthalene and anthracene.

## **UNIT - III: 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, Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis, Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Bischler-Napieralski reaction.

#### UNIT - IV

#### A. Alkaloids

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

#### B. Terpenes

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

- 1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India)Pvt. Ltd. (Pearson Education).
- 2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 3. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 4. Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly & Sons (1976).
- 5. Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- 6. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
- 7. Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P)Ltd. Pub.
- 8. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- 9. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Parakashan (2010).

Total Marks: 50 (Credits: 01)

- 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)

- 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*, 5<sup>th</sup> *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).

Total Marks: 100 (Credits: 03)

#### **UNIT-I: 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.

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.

## **UNIT-II: Electrochemistry-I**

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potential, and applications of electrolysis in metallurgy.

Chemical cells, reversible and irreversible cells with examples. Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells.

# **UNIT-III: Electrochemistry-II**

Electromotive force of a cell, 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.

## UNIT-IV: Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz- Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement by Gouy's method,

- 1. Atkins, P.W & Paula, J.D. *Physical Chemistry*, 10<sup>th</sup> Ed., Oxford University Press (2014).
- 2. Castellan, G. W. *Physical Chemistry* 4<sup>th</sup> Ed., Narosa (2004).
- 3. Mortimer, R. G. *Physical Chemistry 3<sup>rd</sup> Ed.*, Elsevier: NOIDA, UP (2009).
- 4. Barrow, G. M., *Physical Chemistry* 5<sup>th</sup> Ed., Tata McGraw-Hill: New Delhi (2006).
- 5. Engel, T. & Reid, P. Physical Chemistry 3<sup>rd</sup> Ed., Prentice-Hall (2012).
- 6. Rogers, D. W. Concise Physical Chemistry Wiley (2010).
- 7. Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. *Physical Chemistry 4<sup>th</sup> Ed.*, John Wiley & Sons, **k** (2005).

Total Marks: 50 (Credits: 01)

## Conductometry

- I. Determination of cell constant
- II. Determination of equivalent conductance, degree of dissociation and dissociation constant of aweak 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

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

Total Marks: 100 (Credits: 03)

#### UNIT - I

# A. Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides.

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

# B. Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

 $\alpha$ -Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis.

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

#### UNIT - II

## A. Enzymes

Introduction, classification and characteristics of enzymes. Salient features of the active site of enzymes. Mechanism of enzyme action (taking trypsin as an 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).

# B. Lipids

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

#### **UNIT – III: Concept of Energy in Biosystems**

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

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

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

Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Calorific value of food, standard calorific content of food types.

# **UNIT - IV: 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).

- 1. Berg, J.M., Tymoczko, J.L. & Stryer, L. (2006) *Biochemistry*. 6<sup>th</sup> Ed. W.H. Freeman and Co.
- 2. Nelson, D.L., Cox, M.M. & Lehninger, A.L. (2009). *Principles of Biochemistry. IV Edition*. W.H. Freeman and Co.
- 3. Murray, R.K., Granner, D.K., Mayes, P.A. & Rodwell, V.W. (2009) *Harper's Illustrated Biochemistry*. XXVIII edition. Lange Medical Books/ McGraw-Hill.

# CHEM.C-11 (P): ORGANIC CHEMISTRY-IV Lab

Total Marks: 50 (Credits: 01)

- 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 oil or fat.
- 7. Determination of Iodine number of oil/ fat.
- 8. Isolation and characterization of DNA from onion/cauliflower/peas.

- 1. Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
- 2. Arthur, I. V. Quantitative Organic Analysis, Pearson.

## CHEM.C-12 (T): PHYSICAL CHEMISTRY-V: QUANTUM CHEMISTRY & SPECTROSCOPY

Total Marks: 100 (Credits: 03)

## UNIT – I: Quantum Chemistry-I

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; wave functions.

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

Rigid rotator model of rotation of diatomic molecules. Schrödinger equation. Separation of variables.

## UNIT - II: Quantum Chemistry-II

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, and quantization of energy (only final energy expression).

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

## **UNIT – III: 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, degrees of freedom for polyatomic molecules, modes of vibration.

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

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

#### **UNIT – IV: Photochemistry**

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitized reactions, quenching.

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

Total Marks: 50 (Credits: 03)

## **UV-Visible Spectroscopy**

- I. Study the 200-500 nm absorbance spectra of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> (in 0.1 M H<sub>2</sub>SO<sub>4</sub>) and determine the λmax values. Calculate the energies of the two transitions in different units (J molecule<sup>-1</sup>, kJ mol<sup>-1</sup>, cm<sup>-1</sup>, eV).
- II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>.
- 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<sub>4</sub> / KMnO<sub>4</sub> / K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> 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)

- 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 8<sup>th</sup> Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3<sup>rd</sup> Ed.; W.H. Freeman & Co.: New York (2003)

## CHEM.C-13 (T): INORGANIC CHEMISTRY-IV: ORGANOMETALLIC CHEMISTRY

Total Marks: 100 (Credits: 03)

### UNIT – I: Theoretical Principles in Qualitative Analysis (H<sub>2</sub>S Scheme)

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

### **UNIT - II: Organometallic Compounds**

Definition and classification of organometallic compounds on the basis of bond type. Concept of the 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 nuclear carbonyls of 3d series. Structures of mononuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor

Behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain the extent of back bonding.

Zeise's salt: Preparation and structure, evidence of synergic effect.

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).

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

### **UNIT - III: 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.

# UNIT - IV: Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

- 1. Alkene hydrogenation (Wilkinsons Catalyst)
- 2. Hydroformylation (Co salts)
- 3. Wacker Process
- 4. Synthetic gasoline (Fischer Tropsch reaction)

- 1. Svehla, G. Vogel's Qualitative Inorganic Analysis, 7th Edition, Prentice Hall,1996.
- 2. Cotton, F.A.G.; Wilkinson & Gaus, P. L. Basic Inorganic Chemistry 3<sup>rd</sup> Ed.; Wiley India,
- 3. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4<sup>th</sup> Ed.*, Harper Collins 1993, Pearson, 2006.
- 4. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
- 5. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry 3<sup>rd</sup> Ed., John Wiley and Sons, NY, 1994.
- 6. Greenwood, N.N. & Earnshaw, A. *Chemistry of the Elements, Elsevier 2<sup>nd</sup> Ed*, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- 7. Lee, J.D. Concise Inorganic Chemistry 5<sup>th</sup> Ed., John Wiley and sons 2008.
- 8. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- 9. Shriver, D.D. & P. Atkins, *Inorganic Chemistry* 2<sup>nd</sup> Ed., Oxford University Press, 1994.

- 10. Basolo, F. & Pearson, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution*  $2^{nd}$  Ed., John Wiley & Sons Inc; NY.
- 11. Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4<sup>th</sup> Ed., Pearson, 2010.
- 12. Collman, J. P. et al. Principles and Applications of Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
- 13. Crabtree, R. H. *The Organometallic Chemistry of The Transition Metals. j* NewYork, NY: John Wiley, 2000.
- 14. Spessard, G. O. & Miessler, G.L. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

# CHEM.C-13 (P): INORGANIC CHEMISTRY-IV Lab

Total Marks: 50 (Credits: 01)

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 
$$^{2-}$$
, NO  $^{-}$ , S2-, SO<sub>3</sub> $^{2-}$ , S<sub>2</sub>O<sub>3</sub>  $^{2-}$ , CH<sub>3</sub>COO-, F-, Cl-, Br-, I<sup>3</sup>, NO  $^{-}$ , BO  $^{3-}$ , C2O4 $^{2-}$ , PO<sup>3</sup>  $^{3-}$ , NH  $^{+}$ , K+, Pb<sup>2+</sup>, Cu<sup>2+</sup>, Cd<sup>2+</sup>, Bi<sup>3+</sup>, Sn<sup>2+</sup>, Sb<sup>3+</sup>, Fe<sup>3+</sup>, Al<sup>3+</sup>, Cr<sup>3+</sup>, Zn<sup>2+</sup>, Mn<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Ba<sup>2+</sup>, Sr<sup>2+</sup>, Ca<sup>2+</sup>, Mg<sup>2+</sup> Mixtures should preferably contain one interfering anion, **or** insoluble component:

(BaSO<sub>4</sub>, SrSO<sub>4</sub>, PbSO<sub>4</sub>, CaF<sub>2</sub> or Al<sub>2</sub>O<sub>3</sub>) or combination of anions e.g. CO<sub>2</sub>- and SO<sub>3</sub><sup>2</sup>-, NO- and NO<sub>2</sub>- and Br Cl<sup>-</sup> and I<sup>-</sup>, Br <sup>-</sup>and I<sup>-</sup>, NO<sub>3</sub><sup>-</sup> and Br<sup>-</sup>, NO<sub>3</sub><sup>-</sup> and I<sup>-</sup>. Spot tests should be done whenever possible.

- i. Measurement of 10 Dq by the 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  $\lambda$ 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 the substitution method.

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

Total Marks: 100 (Credits: 03)

#### **UNIT – I: Organic** Spectroscopy

General principles: Introduction to absorption and emission spectroscopy.

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

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

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

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

## **UNIT - II: Carbohydrates**

Occurrence, classification and their biological importance.

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, Ring structure of glucose and fructose, 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.

# **UNIT – III: 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 and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein; Natural dyes – structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

#### **UNIT - IV: 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.

Polymerization reactions -Addition and condensation -Mechanism of cationic, anionic and free radical addition polymerization, 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.

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

- 7. McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
- 8. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- 9. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan (2010).
- 10. Kemp, W. Organic Spectroscopy, Palgrave.
- 11. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India Ed. (2015).

Total Marks: 50 (Credits: 01)

- 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.

- 1. Vogel, A.I. Quantitative Organic Analysis, Part 3, Pearson (2012).
- 2. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- 3. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5<sup>th</sup> Ed., Pearson (2012)
- 4. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

Total Marks: 100 (Credits: 03)

#### **UNIT-1**

## A. 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

#### B. Principles of Green Chemistry and Designing a Chemical Synthesis-I

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.
- 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.

# UNIT-II: Principles of Green Chemistry and Designing a Chemical Synthesis-II

- 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.

## UNIT-III: Examples of Green Synthesis/ Reactions and some real-world cases

- 1. Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)
- 2. Microwave-assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave-assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
- 3. Ultrasound-assisted reactions: Sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)
- 4 Surfactants for carbon dioxide replacing smog-producing and ozone-depleting solvents with CO2 for precision cleaning and dry cleaning of garments.
- 5 Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid)made from corn.
- 7 Healthier Fats and Oils by Green Chemistry: Enzymatic Inter esterification for the production of noTrans-Fats and Oils.
- 8 Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.

# **UNIT-IV: Future Trends in Green Chemistry**

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; co-crystal controlled solid state synthesis  $(C_2S_3)$ ; Green chemistry in sustainable development.

- 1. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
- 2. Anastas, P.T. & Warner, J.K.: *Green Chemistry Theory and Practical*, Oxford University Press (1998).
- 3. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
- 4. Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- 5. Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
- 6. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2<sup>nd</sup> Edition, 2010.
- 7. Upasana Bora Sinha, Aspects of Green Chemistry, M.R. Publications, 2014.

Total Marks: 50 (Credits: 01)

# 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 economycan illustrate Green Chemistry.
- Preparation of propene by two methods can be studied
- (I) Triethylamine ion  $+ OH^- \rightarrow propene + trimethylpropene + water <math>H_2SO_4/$
- (II) 1-propanol 
  → propene + water
- Other types of reactions, like addition, elimination, substitution and rearrangement, should also be studied for the calculation of atom economy.

# 4. Use of enzymes as catalysts

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

### 5. Alternative Green solvents

Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice. Mechanochemical solvent-free synthesis of azomethines

# 6. Alternative sources of energy

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

- 1. Anastas, P.T. & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
- 2. Kirchoff, M. & Ryan, M.A. *Greener approaches undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- 3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- 4. 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).
- 5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- 6. Cann, M. C. & Thomas, P. Real world cases in Green Chemistry, American Chemical Society (2008).
- 7. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2<sup>nd</sup> Edition, 2010.
- 8. 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.
- 9. Upasana Bora Sinha, Aspects of Green Chemistry, M.R. Publications, 2014.

# CHEM.C-16 (T): INORGANIC CHEMISTRY V: FUNDAMENTALS OF INORGANIC CHEMISTRY

Total Marks: 100 Credits: 4

## **Unit 1: Acid-Base Concepts**

Acid-Base Concepts: Arrhenius concept - Water ion system; Bronsted-Lowry theory - proton-donor-acceptor system; general theory of solvent system; Lewis's concept - electron-donor-acceptor system; Hard-Soft Acid-Base concept and stability of the complex (A: B); Usanovich concept – positive-negative system.

#### **Unit 2: Non-aqueous Solvents**

Classification of solvents; general properties of ionizing solvents; chemical reactions; Liquid ammonia as solvent; liquid sulfur dioxide as solvent; liquid dinitrogen tetra-oxide; liquid hydrogen fluoride; liquid hydrogen sulfide; liquid hydrogen cyanide; acetic acid; liquid bromine trifluoride; oxyhalides.

# **Unit 3: Chemical Applications of Group Theory**

Symmetry and Structure: Symmetry elements and operations; multiplication of symmetry operations; symmetry point groups with examples from inorganic compounds; groups of very high symmetry; molecular dissymmetry and optical activity; systematic procedure for symmetry classification of molecules and illustrative examples.

Symmetry group theory and its applications: Matrix representation of symmetry operations and groups; reducible and irreducible representations; Great Orthogonality Theorem; character tables. Application of group theory.

# **Unit 4: Nuclear Chemistry**

Basic concepts, models of nuclear structure and stability. Nuclear reactions: nuclear fission, nuclear fusion. Detection and measurement of radioactivity. Application of radioisotopes as tracers in chemical analysis. Isotope effect, isotopic exchange reactions, isotope dilution techniques and radiometric titrations. Radiopharmaceutical, radioimmunoassay and radiation sterilization. Hot atom chemistry.

### **Recommended Books:**

- 1. B. R. Puri, L. R. Sharma, and K. C. Kalia, *Principles of Inorganic Chemistry*, Milestone.
- 2. W. U. Malik, G. D. Tuli, & R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand & Company Ltd.
- 3. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press.
- 4. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press.
- 5. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. Advanced Inorganic Chemistry, John Wiley.
- 6. B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of Inorganic Chemistry, John Wiley & Sons.
- 7. F. A. Cotton. Chemical Applications of Group Theory, John Wiley & Sons.

# CHEM.C-17 (T): ORGANIC CHEMISTRY VI: STEREOCHEMISTRY & ORGANIC TRANSFORMATION REACTIONS

Total Marks: 100 Credits: 4

#### **UNIT-1: Stereochemistry:**

Introduction to geometrical and optical isomerism, concept of chirality, recognition of symmetry elements and chiral structure, R-S nomenclature, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Diastereoisomerism in acyclic and cyclic systems, conformational analysis of simple cyclic(chair and boat cyclohexanes) and acyclic systems, interconversion of Fischer, Newman and sawhorse projections. Threo-erythro nomenclature enantiotopic and diastereotopic atoms, groups and phases, stereo specific and stereo selective synthesis; asymmetric synthesis.

# **UNIT-2: Oxidation Reactions:**

Oxidation with Chromium and Manganese Compound: Oxidation of alcohol, aldehydes, carbon–carbon double bonds, and carbon–hydrogen bonds in organic molecules by Potassium permanganate, manganese dioxide, chromic acid, sodium or potassium dichromate. Oxidation with Peracids and other Peroxides: Oxidation of carbon–carbon double bond, oxidation of carbonyl compound, Baeyer–Villiger oxidation.

## Other methods of oxidation:

Prevost and Woodward hydroxylation, cis- and trans-hydroxylation and glycol cleavage reagents: KMnO<sub>4</sub>, OsO<sub>4</sub>, HIO<sub>4</sub>, Pb(OAc)<sub>4</sub>, Mercuric acetate, selenium dioxide.

## **UNIT-3: Reduction Reactions:**

Heterogeneous hydrogenation: Introduction to catalytic hydrogenation, reduction of different functional groups Homogeneous hydrogenation: Wilkinson's catalyst Dissolving Metal Reduction: Liquid ammonia reduction, Birch Reduction, Clemmensen Reduction Metal Hydride reduction: Reduction with Lithium aluminium hydride, Sodium borohydride, Hydroboration including the reactions of alkyl borane, Meerwein-Pondorf-Verley reduction.

# **UNIT-4: Reactions of Carbonyl Compounds:**

Difference in Reactivity between aldehydes and ketones, stereochemical aspects for determining reactivity; familiar name reactions in carbonyl chemistry: Aldol condensation, Perkin condensation, Reformatsky reaction, Robinson Annulation, Stobbe condensation, Schmidt rearrangement, Beckmann rearrangement, Curtius rearrangement, Dieckmann condensation, Grignard reaction, Hoffmann rearrangement, Lossen rearrangement.

#### Recommended Books:

- 1. W. Carruthers, Modern Methods of Organic Synthesis, Third Ed., Cambridge University Press.
- 2. Organic Reaction Mechanisms, V. K. Ahluwalia, R. K. Parashar, Narosa Publishing House.
- 3. S.H. Pine, Organic Chemistry, McGraw-Hill.
- 4. T.W.G. Solomons Organic Chemistry, John Wiley.
- 5. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International.
- 6. P. S. Kalsi. Stereochemistry, Conformation and Mechanism, New Age.

# CHEM.C-18 (T): PHYSICAL CHEMISTRY VI: THERMODYNAMICS AND CHEMICAL DYNAMICS

Total Marks: 100 Credits: 4

**Unit-1: Chemical Thermodynamics:** Brief resume: concepts of laws of thermodynamics, path and state function, thermodynamic processes, free energy, chemical potential and entropies; Maxwell Relations, Gibbs-Helmholtz, Gibbs-Duhem; solutions- partial molar quantities, partial molar volume and its determination, thermodynamics of mixing, chemical potentials of liquids, liquid mixtures; Activities- solvent activity, solute activity, determination of activity and activity coefficients.

- Unit 2: Non-equilibrium Thermodynamics: Entropy of irreversible processes- Clausius inequality, entropy production and entropy flow; entropy production due to- heat flow, chemical reactions, electrochemical reactions; entropy production in open system; rate of entropy production- generalized forces and fluxes, transformation of the generalized forces and fluxes; phenomenological equations, Onsager's reciprocity relations; electro kinetic phenomena; stationary non-equilibrium states- states of minimum entropy production.
- Unit 3: Chemical Kinetics: Methods of determining rate laws; Collision theory of reaction rates; steric factor; activated complex theory; Arrhenius equation and activated complex theory; ionic reactions kinetic salt effects; steady state kinetics; kinetic control of reactions, homogeneous catalysis.
- **Unit 4: Chemical Dynamics:** Dynamics of chain reactions (hydrogen-bromine reaction; photochemical reactions (hydrogen-bromine and hydrogen-chlorine reactions); general features of fast reactions; study of fast reactions by flow methods; relaxation method, flash photolysis and nuclear magnetic resonance method. Oscillatory reactions (Belousov-Zhabotinsky reaction); kinetics of enzyme reactions

# **Books Suggested:**

- 1. P.W. Atkins, Physical Chemistry, Oxford Uni. Press.
- 2. R. Haase, Thermodynamics of Irreversible Process, (Addition Wesley)
- 3. G.L. Agrawal, Basic Chemical Kinetics, Tata McGraw-Hill.
- 4. K.J. Laidler, Chemical Kinetics, McGraw-Hill.
- **5.** K.L. Kapoor, A Textbook of Physical Chemistry Vol. 1, Mac-Millan.

# CHEM.C-19 (T): RESEARCH METHODOLOGY

Total Marks: 100 Credits: 4

#### **Unit 1: Research Methodology**

Objectives and motivations in research; Characteristics and limitations of research; Components of research work; Criteria of good research, Research process; Types of Research; Fundamental, Pure or Theoretical Research, Applied Research, Descriptive Research, Evaluation Research, Experimental Research, Survey Research, Qualitative Research, Quantitative Research.

#### **UNIT 2: Research Methodology (Contd.)**

Research Design – definition – essentials and types of research design – errors and types of errors in research design. Research problem: Selecting and analyzing the research problem – problem statement formulation – formulation of hypothesis. Variables in Research – Measurement and scaling, Different scales, Construction of instrument, Validity and Reliability of instrument.

## **UNIT 3: Research Ethics**

Publication Ethics: Definition, Introduction and Importance, Conflicts of Interest, Best practices/standards initiatives, and guidelines: COPE, EAME, etc. Plagiarism, Self-Plagiarism, Software for detection of Plagiarism. Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types, complaints and appeals.

# **UNIT 4: Research Ethics (Contd.)**

Ethical issues in research: Code of Ethics in Research, Violation of publication ethics, authorship and contributorship, Intellectual Property Rights, Ethics related to Participants and Researchers: Copyright; Royality, Patent Law, Citation, Acknowledgment. Predatory publishers and journals.

### **Recommended Books:**

- 1. Pagadala Suganda Devi, Research Methodology: A Handbook for Beginners, 2017.
- 2. S. Sachdeva, Research Methodology, 2020.
- 3. Shanti Bhushan Mishra, A Handbook on Research Methodology, 2017.
- 4. C. Neal Stewart Jr., Research Ethics for Scientists: A Companion for Students.
- 5. Ana S. Iltis (ed.), Douglas MacKay (ed.), The Oxford Handbook of Research Ethics, 2024.
- 6. Paul Oliver, The Students' Guide to Research Ethics, 2003.

### CHEM.C-20 (P): ADVANCED LABORATORY COURSE IN CHEMISTRY

Total Marks: 100 Credits: 4

- 1. Learning of laboratory equipment and techniques: Glass Apparatus, Assemblies for Reactions, Distillation, Recrystallization, Determination of melting point, Drying Agents, Cleaning of Apparatus.
- 2. Knowledge of Thin Layer Chromatography (TLC), preparation of TLC plates.
- 3. Extraction of natural products: any one (solasodine, caffeine, nicotine, piperazine, carotenoids etc.).
- 4. Separation and purification of organic compounds from a mixture, using chromatographic techniques, solubility methods, steam distillation, fractional crystallization and sublimation.
- 5. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three-component mixtures and alloys.
- 6. Preparations and characterizations of the following compounds: (Green Chemistry Principle may be applied):
- (i) Potassium trioxalato ferrate (III)
- (ii) Potassium trioxalato chromate (III)
- (iii) Tris(thiourea)copper(I) sulfate
- (iv) Tetraamminecopper(II) sulfate

#### Recommended Books:

- 1. Laboratory manual of organic chemistry, Raj K. Bansal, Wiley-Eastern Ltd.
- 2. Vogel's Textbook of Practical Organic Chemistry, Longman Group UK Ltd.
- 3. Greener approaches to Undergraduate Chemistry Experiments, American Chemical Society.
- 4. Practical Organic Chemistry, F.G. Saunders and B.C. Mann, Orient Longman.
- 5. Aspects of Green Chemistry, Upasana Bora Sinha, M.R. Publishers.
- 6. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. *Vogel's Textbook of Quantitative Chemical Analysis*, Peterson Education.
- 7. G. Marr & B. W. Rockett. Practical Inorganic Chemistry, Van Nostrand.
- 8. G. Pass & H. Sutcliffe. *Practical Inorganic Chemistry*, Chapman & Hill.
- 9. J. Basset, R. C. Denney, G.H. Jeffery & J. Mendham. *Vogel's Textbook of Quantitative Analysis*, English Language Book Society.
- 10. G. W. Parshall (Ed. in Chief). *Inorganic Synthesis*, Vol. 15, McGraw-Hill.

# CHEM.C-21(T): INORGANIC CHEMISTRY VI: CHEMISTRY OF THE ELEMENTS

Total Marks: 100 Credits: 4

### **Unit 1: Chemistry of Main-Group Elements**

Chemical periodicity; allotropy, Allotropy in carbon, phosphorous and sulphur; Structure and bonding in oxyacids of nitrogen, phosphorous, sulphur and halogens; Interhalogens and pseudohalides; Structure and bonding in homo- and heteronuclear molecules; VSEPR theory & Shapes of molecules.

## **Unit 2: Inorganic Cages and Metal Clusters**

Basics of cages and clusters. Wade's rule, Styx notation, electron count in polyhedral boranes. Synthesis, bonding, structures, and properties of boranes and related compounds, phosphazenes. Silicones and compounds with B-N, P-N, and S-N bonds. Introduction to molecular clusters. Main-group clusters. Closo-, nido-, arachno-borane structural paradigm, electron counting rules. Transition-metal clusters. Structure, synthesis and reactivity. Capping rules, isolobal relationships between main-group and transition metal fragments. Main group Transition Metal clusters. Clusters having interstitial main group elements, cubane clusters and Zintl clusters. Clusters in catalysis. Non-stoichiometric oxides: zeolites and clay.

#### **Unit 3: Chemistry of Transition and Inner Transition Elements**

Transition elements: Periodic trends in general properties of transition and inner transition elements, Comparison of properties of first transition series elements with those of second and third transition series elements, Lanthanide contraction, Spectral and magnetic properties, Applications of lanthanide and actinide compounds in industries, Inner transition elements: Spectral and magnetic properties, redox chemistry, analytical applications, Coordination Chemistry: Introduction to coordination chemistry, bonding theories of transition metal complexes, MOT of complexes with and without  $\pi$ -bonding, MO diagrams for octahedral, square planar and tetrahedral complexes.

# **Unit 4: Magnetic Properties of Transition Metal Complexes**

Brief review of different types of magnetic behaviours; Measurement of magnetic susceptibility; Spin-orbit coupling, Quenching of orbital angular momenta, Temperature-independent paramagnetism.

Application of Crystal Field Theory to explain the magnetic properties of coordination compounds. Spin crossover, Structural effects: ionic radii and Jahn-Teller effect; octahedral vs. tetrahedral coordination.

#### **Recommended Books**

- 1. B. R. Puri, L. R. Sharma, and K. C. Kalia, Principles of Inorganic Chemistry, Milestone.
- 2. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi. *Principles of Structure and Reactivity*, Pearson Education.
- 3. F. A. Cotton and G. Wilkinson, *Advanced Inorganic Chemistry*, John Wiley.
- 4. W. U. Malik, G. D. Tuli, & R. D. Madan, Selected Topics in Inorganic Chemistry, S. Chand & Company Ltd.
- 5. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press.
- 6. N. N. Greenwood & A. Earnshaw. Chemistry of the Elements, Pergamon Press.
- 7. F. Basolo& R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern.
- 8. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. Advanced Inorganic Chemistry, John Wiley.
- 9. S. F. A. Kettle, *Physical Inorganic Chemistry*, Spectrum.
- 10. B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of Inorganic Chemistry, John Wiley & Sons.

# CHEM.C-22 (T): ORGANIC CHEMISTRY VII: SYNTHESIS & REACTIONS OF HETEROCYCLIC COMPOUNDS

Total Marks: 100 Credits: 4

**UNIT-1:** (a) Introduction to heterocycles: Hantzsch-Widman Nomenclature; monocyclic, fused and bridged heterocycles; Aliphatic and aromatic heterocycles; Basicity and aromaticity of heterocycles.

- **(b) Small Ring Heterocycles**: Syntheses of aziranes, oxiranes & thiiranes; Ring openings and heteroatom extrusion; Synthesis & reactions of azetidines, oxetanes & thietanes; Strain.
- **UNIT-2: Five membered heterocycles with two heteroatoms**: Structural and chemical properties; Synthesis of pyrazole, isothiazole and isoxazole; Synthesis of imidazoles, thiazoles & oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages; Benzofused analogues.
- **UNIT-3:** (a) Six membered heterocycles with two heteroatoms: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.
- **(b) Bicyclic Heterocycles**: Synthesis of quinolines, isoquinolines, benzofuseddiazines, acridines, phenothiazines, carbazoles and pteridines; Substitution reactions.
- **UNIT-4:** (a) Condensed Five-membered Rings (1 Heteroatom): Synthesis of indole, benzofuran and benzothiophene; Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology.
- (b) Seven-membered Rings: Synthesis & reactions of azepines, oxepines, thiepines & diazepines.

## Recommended Books:

- 1. L. A. Paquette. Modern Heterocyclic Chemistry, W. A. Benjamin.
- 2. I. L. Finar. Organic Chemistry, Vol. II, ELBS.
- 3. J. A. Joule, K. Mills, Heterocyclic Chemistry, John Wiley & Sons.
- 4. Thomas L. Gilchrist, Heterocyclic Chemistry, Longman Ltd.
- 5. Theophil Eicher, S. Hauptmann, *The chemistry of Heterocyclic Chemistry*, Wiley-VCH.
- 5. Katritzky, A. R., Ramsden, C. A., Joule, J. A., and V. V. Zhdankin, *Handbook of Heterocyclic Chemistry*, Pergamon Press.
- 6. A. R. Katritzky & C. W. Rees. *Comprehensive Heterocyclic Chemistry*, Vols. 1-7, Pergamon Press.
- 7. J. Alvarez-Builla, J. J. Vaquero (Editor), J. Barluenga, *Modern Heterocyclic Chemistry*, Wiley-VCH.
- 8. Gupta, Radha R., Kumar, Mahendra, Gupta, Vandana. Heterocyclic Chemistry, Vol; 1,2 and 3, Springer

# CHEM.C-23 (T): PHYSICAL CHEMISTRY VI: QUANTUM MECHANICS AND STATISTICAL THERMODYNAMICS

Total Marks: 100 Credits: 4

# **UNIT 1: General Principles of Quantum Mechanics and Application to Model Systems:**

Introduction, operators and related theorems, uncertainty principle, postulates, properties of wave functions, Schrodinger equation, energy eigenvalue equation, equation of motion and constant of motion, Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential and tunnelling, hydrogen atom.

## **UNIT 2: Theory of Angular Momentum:**

Angular momentum vectors, commutation relations, Chemical bonding in diatomics, elementary concepts of MO and VB theories, Huckel theory of conjugated systems, bond order and charge density calculations, Applications to ethylene, allyl system and butadiene.

# **UNIT 3: Statistical Thermodynamics: Theory and Applications:**

Different types of ensembles, ensemble averaging, thermodynamics of ensemble averaging, Distribution law (Boltzmann statistics), partition function and thermodynamic parameters, relation between molecular and molar partition functions, translational partition functions, rotational partition function for linear and non-linear molecules, vibrational partition function, electronic partition function, reference state of zero energy for evaluating partition function, equilibrium constant in terms of partition function.

## **UNIT 4: Applications of Statistical Thermodynamics:**

Equipartition theorem, heat capacity behaviour of crystals, Introduction to quantum statistics, Distribution law for fermions (Fermi-Dirac statistics) and for bosons (Bose-Einstein statistics), and its applications, Statistical mechanics of imperfect gases, derivation of the virial equation of state of one component gas, significance of virial coefficients, evaluation of second virial coefficient.

## **Books Suggested:**

- 1. D.A. McQuarrie Quantum Chemistry, Oxford University Press.
- 2. I. Levine Quantum Chemistry, Tata McGraw-Hill.
- 4. R. Mc-Weeny Coulson's Valence, ELBS.
- 5. J.N. Murrell, S.F.A. Kettle, J.M. Tedder, Valence Theory, ELBS.
- 6. D. A. McQuarrie and J.D. Simon Physical Chemistry, VIVA Students Ed.
- 7. A.K. Chandra Introductory Quantum Chemistry, Tata McGraw-Hill.
- 8. D. A. McQuarrie. Statistical Mechanics, Viva Books Pvt. Ltd., New Delhi.
- 9. T.L. Hill An introduction to statistical thermodynamics, Dover Publications Inc., New York.
- 10. M.C. Gupta Statistical Thermodynamics, Wiley Eastern.