

# **Syllabus**

**B.Sc.**

**Chemistry**

**W.E.F 2019-2020**



**Raja N.L. Khan Women's College**  
**(Autonomous)**

## Scheme for CBCS Curriculum

### Credit Distribution across Courses (Honours)

Course Type	Total Papers	Credits	
		Theory + Practical	Theory*
Core Courses	14	14*4=56 14*2=28	14*5=70 14*1=14
Discipline Specific Electives	4	4*4=16 4*2=8	4*5=20 4*1=4
Generic Electives	4	4*4=16 4*2=8	4*5=20 4*1=4
Ability Enhancement Language Courses	1(English) 1(ENVS)	1*2=2 2*2=4	1*2=2 2*2=4
Skill Enhancement Courses	2	2*1=2 2*1=2	2*2=4
	26	142	142

### Credit Distribution across Courses (General)

Course Type	Total Papers	Credits	
		Theory + Practical	Theory*
Core Courses	12	12*4=48 12*2=24	12*5=60 12*1=12
Discipline Specific Electives	4	4*4=16 4*2=8	4*5=20 4*1=4
Generic Electives	2	2*4=8 2*2=4	2*5=10 2*1=2
Ability Enhancement Language Courses	1(English) 1(ENVS)	1*2=2 2*2=4	1*2=2 2*2=4
Skill Enhancement Courses	4	4*1=4 4*1=4	4*2=8
	24	122	122

### Course Structure In Hons.

Semester	Sl No.	Name of The Subject	Credit
SEM-I	1	CC1: Physical Chemistry	06
	2	CC2: Inorganic Chemistry	06
SEM-II	3	CC3: Inorganic Chemistry	06
	4	CC4: Organic Chemistry	06
SEM-III	5	CC5: Physical Chemistry	06
	6	CC6: Inorganic Chemistry	06
	7	CC7: Organic Chemistry	06
	8	SEC-I (TBD)	02
SEM-IV	9	CC8: Physical Chemistry	06
	10	CC9: Inorganic Chemistry	06
	11	CC10: Organic Chemistry	06
	12	SEC-II (TBD)	02
SEM-V	13	CC11: Physical Chemistry	06
	14	CC12: Organic Chemistry	06
	15	DSE-I: (TBD)	06
	16	DSE-II (TBD)	06
SEM-VI	17	CC13: Inorganic Chemistry	06
	18	CC14: Organic Chemistry	06
	19	DSE-III: (TBD)	06
	20	DSE-IV (TBD)	06
			112

## **Aims and outcomes of academic programme on B.Sc (Honours) in Chemistry**

### **Educational aims:**

This qualification aims to give:

- a life-long interest in chemistry through modules that are accessible to people with of all educational backgrounds
- an understanding and knowledge of core chemical concepts and principles that underpin the world around us
- practical and problem-solving skills, through the application of standard methodology in chemistry
- an appreciation of the potential and limitations of scientific knowledge in chemistry and an awareness of its environmental, economic and social impact
- a range of transferable skills that will be of value in employment and studies, both within and without the chemical arena
- Support and guidance to develop as an independent learner.

### **Learning outcomes:**

#### **(i) Knowledge and understanding:**

On completion of this qualification, students will have knowledge and understanding of:

- the fundamental concepts, principles, theories, methods and language used in the main branches of chemistry, as well as a basic understanding of its role as the central science across a wider range of scientific disciplines
- the contribution of chemistry to informed debate, and ability to recognize and evaluate different lines of evidence and appreciate the limits of current scientific knowledge
- at least one selected area of chemistry at the forefront of the discipline, informed by literature and independent research.

#### **(ii) Cognitive skills:**

On completion of this qualification, students will be able to:

- select and apply conceptual knowledge and understanding of chemistry to devise and implement strategies, develop and present reasoned arguments, and solve problems in familiar and unfamiliar contexts
- identify, interpret, analyze and critically evaluate chemical information and data from a range of different sources
- apply the methods and techniques they have learned to review, consolidate and extend their knowledge and understanding of chemistry.

#### **(iii) Practical and/or professional skills:**

On completion of this qualification, students will be able to:

- conduct practical investigations in a responsible, safe and ethical manner taking proper account of risk assessment and health and safety regulations
- initiate, design and report on investigations that may involve the acquisition of primary or secondary data
- obtain, record, collate and analyze data derived from practical investigations and interpret and report results on their significance in the light of underlying theory, practical issues and relevant information from other sources
- take personal responsibility to identify goals and organize your tasks effectively, recognizing the necessity for continuing development personally, professionally and in your studies.

#### **(iv) Key skills:**

On completion of this qualification, students will be able to:

- use a range of digital practices and tools to retrieve, use, create, analyze, share and present data, information and knowledge
- select and apply appropriate quantitative methods and tools, appreciating the limits of accuracy and precision in chemical and analytical measurements
- communicate chemical information, data, arguments and ideas accurately and effectively in a style that suits purpose and audience
- work autonomously and interact effectively with others to explore aspects of chemistry, enhance their learning and performance and to achieve joint outcomes.

# Semester-I

Core Course-1 (Credits: Theory-04, Practicals-02)

60L

## CC1T: Physical Chemistry-I

**Course objectives and expected outcome:** The kinetic theory of gases explains the three macroscopic properties of a gas in terms of the microscopic nature of atoms and molecules making up the gas. Usually, the physical properties of solids and liquids can be described by their size, shape, mass, volume etc. However, when we talk about gases, they have no definite shape, size while mass and volume are not directly measurable. The Kinetic theory of gases is useful and can be applied in this case.

With the help of the kinetic theory of gases, the physical properties of any gas can be defined generally in terms of three measurable macroscopic properties.

This course also deals with the fundamentals of Thermodynamics including thermodynamic systems and properties, relationships among the thermos-physical properties, the laws of thermodynamics and applications of these basic laws in thermodynamic systems.

After successful completion of this course the students will be able to:

1. Explain fundamental concepts relevant to thermodynamics.
2. Explain the concepts of work, power, and heat in thermodynamics; determine work and heat sign conventions; determine work involved with moving boundary systems (graphical and analytical methods).
3. Explain the first law of thermodynamics for a closed system.
4. Perform energy analysis of refrigeration and heat pump thermodynamic cycles.
5. Determine thermodynamic properties of pure substances.
6. Apply the first law of thermodynamics for a control volume, including with turbines, compressors, nozzles, diffusers, heat exchangers, and throttling devices.
7. Explain the second law of thermodynamics, including why it is necessary, how it is defined (Kelvin-Planck and Clausius), the nature of irreversibility, and the Carnot cycle.
8. Explain the concept of entropy, including the Clausius Inequality.

Chemical kinetics is the study of the rates and the mechanism of chemical reactions. Commonly the measure of how fast the products are formed and the reactants consumed is given by the rate values.

The study of chemical kinetics has been highly useful in determining the factors that influence the rate, maximum yield and conversion in industrial processes. The mechanism or the sequence of steps by which the reaction occurs can be known. It is also useful in selecting the optimum conditions for maximum rate and yield of the chemical process.

### Unit:-1: Kinetic Theory and Gaseous state

20L

**Kinetic Theory of gases:** Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Wall collision and rate of effusion

**Maxwell's distribution of speed and energy:** Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy  $\geq$  , Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

**Real gas and virial equation:** Deviation of gases from ideal behavior; compressibility

factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dieterici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

### **Unit:-2: Chemical Thermodynamics**

**25L**

Zeroth and 1<sup>st</sup> law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy 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; Joule's experiment and its consequence.

Thermochemistry: Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin — Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of  $\int dQ/T$  and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; Auxiliary state functions ( $G$  and  $A$ ) and their variation with  $T$ ,  $P$  and  $V$ . Criteria for spontaneity and equilibrium.

Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations

### **Unit:-3: Chemical kinetics**

**15L**

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and  $n$ th order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)

Role of  $T$  and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation — explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot, turn-over number

Autocatalysis; periodic reactions

## Reference Books

1. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
5. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
6. Maron, S. & Prutton *Physical Chemistry*
7. Ball, D. W. *Physical Chemistry*, Thomson Press
8. Mortimer, R. G. *Physical Chemistry*, Elsevier
9. Laidler, K. J. *Chemical Kinetics*, Pearson
10. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*
11. Rakshit, P.C., *Physical Chemistry* Sarat Book House
12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
13. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
14. Clauze & Rosenberg, *Chemical Thermodynamics*

## **CC1P : Physical Chemistry LAB-I**

**45L**

**Course objectives and expected outcome:** The course provides training in advanced physical chemistry laboratory techniques. The experiments are guided by demonstrators and are designed both to illustrate the applications of theory covered in the Chemical Physics and lecture courses, and to introduce typical instrumentation. On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.
2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.
8. Developed skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
9. Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

Experiment 1: Determination of pH of unknown solution (buffer), by color matching method

Experiment 2: Determination of heat of neutralization of a strong acid by a strong base

Experiment 3: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 4: Study of kinetics of decomposition of H<sub>2</sub>O<sub>2</sub>

Experiment 5: Determination of heat of solution of oxalic acid from solubility measurement

## Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

## Core Course-2 (Credits: Theory-04, Practicals-02)

### CC2T:INORGANIC CHEMISTRY-I 60L

**Course objectives and expected outcome:** Upon successful completion students should be able to apply the fundamental principles of measurement, matter, atomic theory, chemical periodicity, general chemical reactivity and solution chemistry to subsequent courses in science.

#### Unit-1: Extra nuclear Structure of atom

16L

Bohr's theory, its limitations and atomic spectrum of hydrogen atom; Sommerfeld's Theory. 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. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Pauli's Exclusion Principle, Hund's rules and multiplicity, Exchange energy, Aufbau principle and its limitations, Ground state Term symbols of atoms and ions for atomic number up to 30.

#### Unit-2: Chemical periodicity

14L

Modern IUPAC Periodic table, Effective nuclear charge, screening effects and penetration, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii, lanthanide contraction. Ionization potential, electron affinity and electronegativity (Pauling's, Mulliken's and Allred-Rochow's scales) and factors influencing these properties, group electronegativities. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements. Secondary periodicity, Relativistic Effect, Inert pair effect.

#### Unit-3: Acid-Base reactions

14L

Acid-Base concept: Arrhenius concept, theory of solvent system (in H<sub>2</sub>O, NH<sub>3</sub>, SO<sub>2</sub> and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling's rules. Lux-Flood concept, Lewis concept, group characteristics of Lewis acids, solvent levelling and differentiating effects. Thermodynamic acidity parameters, Drago-Wayland equation. Superacids, Gas phase acidity and proton affinity; HSAB principle. Acid-base equilibria in aqueous solution (Proton transfer equilibria in water), pH, buffer. Acid-base neutralisation curves; indicator, choice of indicators.

#### Unit-4: Redox Reactions and precipitation reactions

16L

Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation (without derivation). Influence of complex formation, precipitation and change of pH on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer and Frost diagrams) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples). Theoretical principles involved in analysis of cations and anions and Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after group II.

#### Reference Books

1. Lee, J. D. *Concise Inorganic Chemistry*, 5<sup>th</sup> Ed., Wiley India Pvt. Ltd., 2008.
2. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970.
3. Day, M.C. and Selbin, J. *Theoretical Inorganic Chemistry*, ACS Publications, 1962.
4. Atkin, P. *Shriver & Atkins' Inorganic Chemistry*, 5<sup>th</sup> Ed., Oxford University Press (2010).
5. Cotton, F.A., Wilkinson, G. and Gaus, P.L., *Basic Inorganic Chemistry 3<sup>rd</sup> Ed.*; Wiley



India.

6. Sharpe, A.G., *Inorganic Chemistry*, 4<sup>th</sup> Indian Reprint (Pearson Education) 2005.
7. 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.
8. Atkins, P.W. & Paula, J. *Physical Chemistry*, Oxford Press, 2006.
9. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).
10. Winter, M. J., The Orbitron, <http://winter.group.shef.ac.uk/orbitron/> (2002). An illustrated gallery of atomic and molecular orbitals.
11. Burgess, J., *Ions in solution: basic principles of chemical interactions*. Ellis Horwood (1999).

### CC2P: Inorganic Chemistry LAB-I

30L

**Course objectives and expected outcome:** Facilitate the learner to experience in qualitative semi micro analysis of mixtures containing four radicals and to understand the chemistry of different reactions and to assign the most probable composition.

#### Qualitative semi micro analysis

Qualitative semi micro analysis of mixtures containing four radicals. Emphasis to be given to the understanding of the chemistry of different reactions and to assign the most probable composition.

Cation Radicals:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}/\text{Mn}^{4+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Co}^{2+}/\text{Co}^{3+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Bi}^{3+}$ ,  $\text{Sn}^{2+}/\text{Sn}^{4+}$ ,  $\text{As}^{3+}/\text{As}^{5+}$ ,  $\text{Sb}^{3+}/\text{Sb}^{5+}$ ,  $\text{NH}_4^+$ ,  $\text{Mg}^{2+}$ .

Anion Radicals:  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{BrO}_3^-$ ,  $\text{I}^-$ ,  $\text{IO}_3^-$ ,  $\text{SCN}^-$ ,  $\text{S}^{2-}$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{AsO}_4^{3-}$ ,  $\text{BO}_3^{3-}$ ,  $\text{CrO}_4^{2-}$ ,  $\text{Cr}_2\text{O}_7^{2-}$ ,  $\text{Fe}(\text{CN})_6^{4-}$ ,  $\text{Fe}(\text{CN})_6^{3-}$ .

Insoluble Materials:  $\text{Al}_2\text{O}_3(\text{ig})$ ,  $\text{Fe}_2\text{O}_3(\text{ig})$ ,  $\text{Cr}_2\text{O}_3(\text{ig})$ ,  $\text{SnO}_2$ ,  $\text{SrSO}_4$ ,  $\text{BaSO}_4$ ,  $\text{CaF}_2$ ,  $\text{PbSO}_4$

#### Reference Books

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

## Semester-II

### Core Course-3 (Credits: Theory-04, Practicals-02)

#### CC3T: INORGANIC CHEMISTRY-II 60L

**Course objectives and expected outcome:** Upon successful completion students should be able to: know the bonding fundamentals for both ionic and covalent compounds, including electronegativities, bond distances and bond energies using MO diagrams and thermodynamic data and to predict geometries of simple molecules. They will also acquire the basic knowledge of nuclear structure, stable and unstable atomic nuclei, nuclear reactions and different modes of radioactive decay and also methods for measurements of radioactivity. The fundamentals of radiochemistry, isotopic chemistry, radiation chemistry and the applications of these in measuring technology, kinetics, radical chemistry, biotechnology and materials and process technology.

#### Unit-1: Chemical Bonding-I

20L

1. *Ionic bond*: General characteristics, types of ions, size effects, radius ratio rule and its application and 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. Defects in solids (elementary idea). Solubility energetics of dissolution process.

2. *Covalent bond*: Polarizing power and polarizability, ionic potential, Fajan's rules. Lewis structures, formal charge. Valence Bond Theory. The hydrogen molecule (Heitler-London approach), directional character of covalent bonds, hybridizations, equivalent and non-

equivalent hybrid orbitals, Bent's rule, Dipole moments, VSEPR theory, shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry) and multiple bonding ( $\sigma$  and  $\pi$  bond approach).

### Unit-2: Chemical Bonding-II

30L

1. Molecular orbital concept of bonding (The approximations of the theory, Linear combination of atomic orbitals (LCAO)) (elementary pictorial approach): sigma and pi-bonds and delta interaction, multiple bonding. Orbital designations: *gerade*, *ungerade*, HOMO, LUMO. Orbital mixing,. MO diagrams of  $H_2$ ,  $Li_2$ ,  $Be_2$ ,  $B_2$ ,  $C_2$ ,  $N_2$ ,  $O_2$ ,  $F_2$ , and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO,  $NO^+$ ,  $CN^-$ , HF,  $BeH_2$ ,  $CO_2$  and  $H_2O$ . Bond properties: bond orders, bond lengths.
2. *Metallic Bond*: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.
3. *Weak Chemical Forces*: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Intermolecular forces: Hydrogen bonding (theories of hydrogen bonding, valence bond treatment), receptor-guest interactions, Halogen bonds. Effects of chemical force, melting and boiling points.

### Unit-3: Radioactivity

10L

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes. Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

#### Suggested Readings :

1. Lee, J. D. *Concise Inorganic Chemistry*, 5<sup>th</sup> Ed., Wiley India Pvt. Ltd., 2008.
2. 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.
3. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970.
4. Porterfield, H. W., *Inorganic Chemistry*, Second Edition, Academic Press, 2005.
5. Purecell, K.F. and Kotz, J.C., *An Introduction to Inorganic Chemistry*, Saunders: Philadelphia, 1980.
6. Cotton, F.A., Wilkinson, G., & Gaus, P.L. *Basic Inorganic Chemistry* 3<sup>rd</sup> Ed.; Wiley India.
7. Gillespie, R. J. and Hargittai, I., *The VSEPR Model of Molecular Geometry*, Prentice Hall (1992).
8. Albright, T., *Orbital interactions in chemistry*, John Wiley and Sons (2005).
9. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).
10. Miessler, G. L., Fischer, P. J., Tarr, D. A., *Inorganic Chemistry*, Pearson, 5<sup>th</sup> Edition.
11. Kaplan, I., *Nuclear Physics*, Addison-Wesley Publishing Company Inc. London, 1964.
12. Friedlander, G., Kennedy, J. W., Macias, E. S. And Miller, J. M., *Nuclear and Radiochemistry*, Wiley, 1981.

### CC3P: Inorganic Chemistry LAB-II

45L

**Course objectives and expected outcome:** Facilitate the learner to make solutions of various molar concentrations. This may include: The concept of the mole; Converting moles to grams; Converting grams

to moles; Defining concentration; Dilution of Solutions; Making different molar concentrations. They will also experiences in different type of titration like acid-base, oxidation-reduction titration.

#### **Acid and Base Titrations:**

1. Estimation of carbonate and hydroxide present together in mixture
2. Estimation of carbonate and bicarbonate present together in a mixture.
3. Estimation of free alkali present in different soaps/detergents.

#### **Oxidation-Reduction Titrimetric**

1. Estimation of Fe(II) using standardized  $\text{KMnO}_4$  solution
2. Estimation of oxalic acid and sodium oxalate in a given mixture
3. Estimation of Fe(II) and Fe(III) in a given mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$  solution.
4. Estimation of Fe(III) and Mn(II) in a mixture using standardized  $\text{KMnO}_4$  solution
5. Estimation of Fe(III) and Cu(II) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .
6. Estimation of Fe(III) and Cr(III) in a mixture using  $\text{K}_2\text{Cr}_2\text{O}_7$ .

#### **Reference Books**

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

### **Core Course-4 (Credits: Theory-04, Practicals-02)**

#### **CC4T - : ORGANIC CHEMISTRY-I**

**60L**

**Course objectives and expected outcome:** Working through this course, students are expected to apply their knowledge to problem-solve, deduce structures, Bonding geometries of carbon compounds and representation of molecules, concept of chirality, optical activity of chiral compounds and symmetry, and synthesize simple organic molecules using the studied reactions. Relationships between organic chemistry and other disciplines are noted.

#### **Basics of Organic Chemistry:**

#### **Unit-I: Bonding and Physical**

##### **Properties 28L**

*Valence Bond Theory:* concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding ( $\text{sp}^3$ ,  $\text{sp}^2$ ,  $\text{sp}$ : C-C, C-N & C-O systems and *s-cis* and *s-trans* geometry for suitable cases).

*Electronic displacements:* inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.

*MO theory:* qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ ,  $n$  — MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of  $\pi$  MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about  $\alpha$  and  $\beta$ ; measurement of delocalization energies in terms of  $\beta$  for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

*Physical properties:* influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's

strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.

## Unit-II: General Treatment of Reaction Mechanism I

10L

*Mechanistic classification:* ionic, radical and pericyclic (definition and example);

reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.

*Reactive intermediates:* carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

## Unit-III: Stereochemistry I

22L

*Bonding geometries of carbon compounds and representation of molecules:* tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations.

*Concept of chirality and symmetry:* symmetry elements and point groups ( $C_{\infty v}$ ,  $C_{nh}$ ,  $C_{nv}$ ,  $C_n$ ,  $D_{\infty h}$ ,  $D_{nh}$ ,  $D_{nd}$ ,  $D_n$ ,  $S_n$  ( $C_s$ ,  $C_i$ )); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).

*Relative and absolute configuration:* D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/Z- isomerisms.

*Optical activity of chiral compounds:* optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates); resolution of acids, bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

### Reference Books

1. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
2. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
3. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
4. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
5. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
6. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
7. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
8. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

9. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
10. Fleming, I. *Molecular Orbitals and Organic Chemical Reactions*, Reference/Student Edition, Wiley, 2009.
11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.

#### CC4P – ORGANIC CHEMISTRY LAB- I

45L

**Course objectives and expected outcome:** Facilitate the learner to separate the components based upon solubility, by using common laboratory reagents, to purify the separated components by crystallization and determination of its melting point, to identify the pure organic compounds.

**1. Separation**, based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, etc., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture may be of the following types: Benzoic acid/*p*-Toluidine; *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotoluene/*p*-Anisidine; etc.

**2. Determination of boiling point** of common organic liquid compounds e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160 °C]

#### 3. Identification of a Pure Organic Compound

*Solid compounds:* oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid

*Liquid Compounds:* formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

#### Reference Books

1. Bhattacharyya, R. C. *A Manual of Practical Chemistry*.
2. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, CBS Publishers and Distributors.
3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
4. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012).
5. Dutta, S, *B. Sc. Honours Practical Chemistry*, Bharati Book Stall.

## Semester-III

**Core Course : 5 Credit: 06 (Theoretical:04;Practical:02)**

**CC5T: Physical Chemistry-II 60L**

**Course objectives and expected outcome:** Facilitate the learner to know about the transport phenomenon with respect to viscosity and conductance. They will gain the concept of Chemical cells. This course will also deliver the students to experience the application of thermodynamics in chemical equilibrium and phase equilibrium.

**Unit:-I: Transport processes 20L**

Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general

form), different examples of transport properties

Viscosity: General features of fluid flow (streamline flow and turbulent flow); Newton's equation, viscosity coefficient; Poiseuille's equation; principle of determination of viscosity coefficient of liquids by falling sphere method; Temperature variation of viscosity of liquids and comparison with that of gases

Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye-Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations

Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule

**Unit:-II: Electromotive Force:**

12L

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

**Unit:-III: Applications of Thermodynamics – I**

28L

Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential ( $\mu$ ) with temperature and pressure; Gibbs-Duhem equation; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S H and V during mixing for binary solutions

Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of  $K_p$ ,  $K_c$  and  $K_x$ ; van't Hoff's reaction isobar and isochore from different standard states; Shifting of equilibrium due to change in external parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle and its derivation

Nernst's distribution law; Application- (finding out  $K_{eq}$  using Nernst dist law for  $\text{KI} + \text{I}_2 = \text{KI}_3$  and dimerization of benzene)

Chemical potential and other properties of ideal substances- pure and mixtures: a) Pure ideal gas-its Chemical potential and other thermodynamic functions and their changes during a change of; Thermodynamic parameters of mixing; Chemical potential of an ideal gas in an ideal gas mixture; Concept of standard states and choice of standard states of ideal gases

b) Condensed Phase — Chemical potential of pure solid and pure liquids, Ideal solution — Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution; Choice of standard states of solids and liquids

### Reference Books:

1. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
5. Rakshit, P.C., *Physical Chemistry*, Sarat Book House
6. Moore, W. J. *Physical Chemistry*, Orient Longman
7. Mortimer, R. G. *Physical Chemistry*, Elsevier
8. Denbigh, K. *The Principles of Chemical Equilibrium* Cambridge University Press
9. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
10. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
11. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
12. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics: Basic Concepts and Methods* Wiley
13. Glasstone, S. *An Introduction to Electrochemistry*, East-West Press

### CC5P: Physical Chemistry-II Lab

45L

**Course objectives and expected outcome:** The course provides training in advanced physical chemistry laboratory techniques. The experiments are guided by demonstrators and are designed both to illustrate the applications of theory covered in the Chemical Physics and lecture courses, and to introduce typical instrumentation. On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.
2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.
8. Developed skills in the conductometric titration.
9. Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

**Experiment 1:** Study of viscosity of unknown liquid (glycerol, sugar) with respect to water

**Experiment 2:** Determination of partition coefficient for the distribution of  $I_2$  between water and  $CCl_4$

**Experiment 3:** Determination of  $K_{eq}$  for  $KI + I_2 = KI_3$ , using partition coefficient between water and  $CCl_4$

**Experiment 4:** Conductometric titration of an acid (strong, weak/ monobasic, dibasic)

against base strong

**Experiment 5:** Study of saponification reaction conductometrically

**Experiment 6:** Verification of Ostwald's dilution law and determination of  $K_a$  of weak acid

**Suggested Readings :**

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

**Core Course-6 (Credits: Theory-04, Practicals-02)**

**CC6T:INORGANIC CHEMISTRY-III 60L**

**Course objectives and expected outcome:** Students will be able to gain idea about the general principles of metallurgy, chemistry of s and p block elements, noble gases, Inorganic Polymers and Coordination Chemistry.

**Unit:-I: General Principles of Metallurgy**

**17L**

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.

**Unit:-II: Chemistry of s and p Block Elements**

**31L**

Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Beryllium hydrides and halides. Boric acid and borates, boron nitrides, borohydrides (diborane) and graphitic compounds, silanes, Oxides and oxoacids of nitrogen, phosphorus, sulphur and chlorine. Peroxo acids of sulphur, sulphur-nitrogen compounds, interhalogen compounds, polyhalide ions, pseudohalogens, fluorocarbons and basic properties of halogens.

**Noble Gases:**

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of  $\text{XeF}_2$ ,  $\text{XeF}_4$  and  $\text{XeF}_6$ ; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for  $\text{XeF}_2$  and  $\text{XeF}_4$ ). Xenon-oxygen compounds. Molecular shapes of noble gas compounds (VSEPR theory).

**Inorganic Polymers:**

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



Coordinate bonding: double and complex salts. Werner's theory of coordination complexes, Classification of ligands, Ambidentate ligands, chelates, Coordination numbers, IUPAC nomenclature of coordination complexes (up to two metal centers), Isomerism in coordination compounds, constitutional and stereo isomerism, Geometrical and optical isomerism in square planar and octahedral complexes.

**Suggested Readings:**

1. 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.
2. Greenwood, N.N. & Earnshaw A. *Chemistry of the Elements*, Butterworth-Heinemann, 1997.
3. Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., *Advanced Inorganic Chemistry 6<sup>th</sup> Ed.* 1999., Wiley.
4. Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4<sup>th</sup> Ed.*, Pearson, 2010.
5. Purecell, K.F. and Kotz, J.C., *An Introduction to Inorganic Chemistry*, Saunders: Philadelphia, 1980.
6. Mingos, D.M.P., *Essential trends in inorganic chemistry*. Oxford University Press (1998).

**CC6P: LAB****45L**

**Course objectives and expected outcome:** Facilitate the learner to about complexometric titration and they will also gain the concept in laboratory how the inorganic complexes are formed.

**Practical: Complexometric titration**

1. Zn(II)
2. Zn(II) in a Zn(II) and Cu(II) mixture.
3. Ca(II) and Mg(II) in a mixture.
4. Hardness of water.

**Inorganic preparations**

1.  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6/\text{ClO}_4$
2. *Cis* and *trans*  $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
3. Potassium diaquadioxalatochromate(III)
4. Tetraamminecarbonatocobalt (III) ion
5. Potassium tris(oxalato)ferrate(III)
6. Tris-(ethylenediamine) nickel(II) chloride.
7.  $[\text{Mn}(\text{acac})_3]$  and  $[\text{Fe}(\text{acac})_3]$  (acac= acetylacetonate)

**Suggested Readings:**

1. Mendham, J., A. I. *Vogel's Quantitative Chemical Analysis* 6th Ed., Pearson, 2009.
2. *Inorganic Synthesis*, Vol. 1-10.

**Core Course: 7 Credit: 06 (Theoretical: 04;Practical:02)**

**CC7T:ORGANIC CHEMISTRY-II 60L**

**Course objectives and expected outcome:** Facilitate the learner to know about stereochemistry, reaction thermodynamics, concept of organic acids and bases, tautomerism and reaction kinetics.

**Unit:-I: Stereochemistry II**

**27L**

*Chirality arising out of stereoaxis:* stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkyldenecycloalkanes and biphenyls; related configurational descriptors ( $R_a/S_a$  and  $P/M$ ); atropisomerism; racemisation of chiral biphenyls; *buttressing* effect.

*Concept of prostereoisomerism:* prostereogenic centre; concept of (*pro*)<sup>n</sup>-*chirality*: topicity of ligands and faces (elementary idea); *pro-R/pro-S*, *pro-E/pro-Z* and *Re/Si* descriptors; *pro-r* and *pro-s* descriptors of ligands on propseudoasymmetric centre.

*Conformation:* conformational nomenclature: eclipsed, staggered, *gauche*, *syn* and *anti*; dihedral angle, torsion angle; Klyne-Prelog terminology;  $P/M$  descriptors; energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; *butane gauche* interaction; conformational analysis of ethane, propane, *n*-butane, 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (*s-cis* and *s-trans*).

**Unit:-II: General Treatment of Reaction Mechanism II**

**18L**

*Reaction thermodynamics:* free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.

*Concept of organic acids and bases:* effect of structure, substituent and solvent on acidity and basicity; proton sponge; gas-phase acidity and basicity; comparison between nucleophilicity and basicity; HSAB principle; application of thermodynamic principles in acid-base equilibria.

*Tautomerism:* prototropy (keto-enol, nitro - *aci*-nitro, nitroso-oximino, diazo-amino and enamine-imine systems); valence tautomerism and ring-chain tautomerism; composition of the equilibrium in different systems (simple carbonyl; 1,2- and 1,3-dicarbonyl systems, phenols and related systems), factors affecting keto-enol tautomerism; application of thermodynamic principles in tautomeric equilibria.

*Reaction kinetics:* rate constant and free energy of activation; concept of order and molecularity; free energy profiles for one-step, two-step and three-step reactions; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect: primary and secondary kinetic isotopic effect ( $k_H/k_D$ ); principle of microscopic reversibility; Hammond's postulate.

**Unit:-III: Chemistry of alkenes and alkynes**

**15L**

*Addition to C=C:* mechanism (with evidence wherever applicable), reactivity, regioselectivity (Markownikoff and anti-Markownikoff additions) and stereoselectivity;

reactions: hydrogenation, halogenations, iodolactonisation, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, epoxidation, *syn* and *anti*-hydroxylation, ozonolysis, addition of singlet and triplet carbenes; electrophilic addition to diene (conjugated dienes and allene); radical addition: HBr addition; mechanism of allylic and benzylic bromination in competition with brominations across C=C; use of NBS; Birch reduction of benzenoid aromatics; interconversion of *E* - and *Z* - alkenes; contra-thermodynamic isomerization of internal alkenes.

*Addition to C≡C (in comparison to C=C):* mechanism, reactivity, regioselectivity (Markownikoff and anti-Markownikoff addition) and stereoselectivity; reactions: hydrogenation, halogenations, hydrohalogenation, hydration, oxymercuration-demercuration, hydroboration-oxidation, dissolving metal reduction of alkynes (Birch); reactions of terminal alkynes by exploring its acidity; interconversion of terminal and non-terminal alkynes.

### Elimination reactions

**Elimination reactions:** E1, E2, E1cB and Ei (pyrolytic *syn* eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination; importance of Bredt's rule relating to the formation of C=C.

### Reference Books

1. Clayden, J., Greeves, N., Warren, S. *Organic Chemistry*, Second edition, Oxford University Press 2012.
2. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
3. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
4. Carey, F. A. & Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
5. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press, 2008.
6. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
7. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
8. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
9. Finar, I. L. *Organic Chemistry (Volume 1)* Pearson Education.
10. Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry*, John Wiley & Sons, Inc.
11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.
13. Maskill, H., *Mechanisms of Organic Reactions*, Oxford Chemistry Primer, Oxford University Press.

### CC7P CHEMISTRY (LAB)

45L

**Course objectives and expected outcome:** Facilitate the learner to calculate percentage yield based upon isolated yield (crude) and theoretical yield.

### Organic Preparations

A. The following reactions are to be performed, noting the yield of the crude product:

1. Nitration of aromatic compounds
2. Condensation reactions
3. Hydrolysis of amides/imides/esters
4. Acetylation of phenols/aromatic amines
5. Benzoylation of phenols/aromatic amines
6. Side chain oxidation of aromatic compounds
7. Diazo coupling reactions of aromatic amines
8. Bromination of anilides using green approach (Bromate-Bromide method)
9. Redox reaction including solid-phase method
10. Green 'multi-component-coupling' reaction
11. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline

**Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.**

B. Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.

C. Melting point of the purified product is to be noted.

#### Reference Books

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 1: *Small scale Preparations*, CBS Publishers and Distributors.
2. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N. University of Calcutta, 2003.
3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
4. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed. Pearson (2012).
5. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
6. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.

## Skill Enhancement Course (SEC)

### SEC-I (Credit:2) Any one of the following

**1. SEC: Analytical Clinical Biochemistry**

**Credits:**

**02 SEC-T: Analytical Clinical Biochemistry**

**Credits:**

**01**

**Course objectives and expected outcome:** Facilitate the learner to understand the structures, properties and functions of carbohydrates, lipids and proteins and to gain the idea about diagnostic approach by blood/ urine analysis.

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

Review of concepts studied in the core course:

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

**Proteins:** Classification, biological importance; Primary and secondary and tertiary structures of proteins:  $\alpha$ -helix and  $\beta$ -pleated sheets, Isolation, characterization, denaturation of proteins.

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

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

Biochemistry of peptide hormones.

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

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

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

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

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

## **SEC-1P: Analytical Clinical Biochemistry**

**Credits: 01**

**Course objectives and expected outcome:** Facilitate the learner to identify and estimate carbohydrates, proteins and lipids in laboratory.

### **Practicals:**

Identification and estimation of the following:

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

### **Reference Books:**

- Cooper, T.G. *Tool of Biochemistry*. Wiley-Blackwell (1977).
- Wilson, K. & Walker, J. *Practical Biochemistry*. Cambridge University Press (2009).
- Varley, H., Gowenlock, A.H & Bell, M.: *Practical Clinical Biochemistry*, Heinemann, London (1980).
- Devlin, T.M., *Textbook of Biochemistry with Clinical Correlations*, John Wiley & Sons, 2010.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.
- Talwar, G.P. & Srivastava, M. *Textbook of Biochemistry and Human Biology*, 3rd Ed. PHI Learning.
- Nelson, D.L. & Cox, M.M. *Lehninger Principles of Biochemistry*, W.H. Freeman, 2013.
- O. Mikes, R.A. Chalmers: *Laboratory Handbook of Chromatographic Methods*, D. Van Nostrand & Co., 1961.

## 2. SEC: Pharmaceutical Chemistry

**Credits: 02**

### SEC-T: Pharmaceutical Chemistry

**Credits: 01**

**20L**

**Course objectives and expected outcome:** Facilitate the learner to understand about the structures, properties and functions of drugs and pharmaceuticals and to gain the idea about fermentation.

### Drugs & Pharmaceuticals

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

### Fermentation

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

### SEC-1P: Pharmaceutical Chemistry

**20L**

**Credits: 01**

**Course objectives and expected outcome:** Facilitate the learner to gain knowledge about the preparation of drugs like aspirin in laboratory.

### 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.

### **3. SEC: BASIC ANALYTICAL CHEMISTRY      30L      Credits 02**

#### **SEC-T: BASIC ANALYTICAL CHEMISTRY**

**Credits 01**

Course objectives and expected outcome: Facilitate the learner to understand about the Concept of sampling and importance of accuracy, precision and sources of error in analytical measurements in analytical chemistry and to analyze the nature of soil, water, food products. They also know application of chromatography and ion exchange method.

#### **Course Contents:**

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

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

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

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

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

**Ion-exchange:** Column, ion-exchange chromatography etc.

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

#### **SEC-P: Practical**

**20L**

**Credits 01**

Course objectives and expected outcome: Facilitate the learner to understand to analyze the nature of soil, water, food products. They will also find application of chromatography and ion exchange method by doing practical in laboratory. They will also gain the knowledge about cosmetic products like deodorants, antiperspirant, talcum powder etc.

#### **A:**

1. Determination of pH of soil samples.
2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.
3. Determination of pH, acidity and alkalinity of a water sample.
4. Determination of dissolved oxygen (DO) of a water sample.

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

**B:**

**Suggested Applications (Any one):**

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

**C:Suggested Instrumental demonstrations:**

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

**Suggested Readings:**

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



# Semester-IV

**Core Course: 8 Credit: 06 (Theoretical: 04; Practical: 02)**

**Core Course: 5**

**CC8: Physical Chemistry-III 60L**

**Course objectives and expected outcome:** Facilitate the learner to understand Colligative properties, phase rule, electrical properties of molecules and quantum chemistry.

**Unit-I: 20L**

**Application of Thermodynamics – II**

Colligative properties: Vapour pressure of solution; Ideal solutions, ideally diluted solutions and colligative properties; Raoult's law; 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; Abnormal colligative properties

Phase rule: Definitions of phase, component and degrees of freedom; Phase rule and its derivations; Definition of phase diagram; Phase diagram for water, CO<sub>2</sub>, Sulphur

First order phase transition and Clapeyron equation; Clausius-Clapeyron equation - derivation and use; Liquid vapour equilibrium for two component systems; Phenol-water system

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

Binary solutions: Ideal solution at fixed temperature and pressure; Principle of fractional distillation; Duhem-Margules equation; Henry's law; Konowaloff's rule; Positive and negative deviations from ideal behavior; Azeotropic solution; Liquid-liquid phase diagram using phenol- water system; Solid-liquid phase diagram; Eutectic mixture

**Unit-II: Electrical Properties of molecules**

**10L**

Ionic equilibria: Chemical potential of an ion in solution; Activity and activity coefficients of ions in solution; Debye-Huckel limiting law-brief qualitative description of the postulates involved, qualitative idea of the model, the equation (without derivation) for ion-ion atmosphere interaction potential. Estimation of activity coefficient for electrolytes using Debye-Huckel limiting law; Derivation of mean ionic activity coefficient from the expression of ion-atmosphere interaction potential; Applications of the equation and its limitations

Dipole moment and polarizability: Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules; Clausius-Mosotti equation and Debye equation (both without derivation) and their application; Determination of dipole moments

**Unit-III: Quantum Chemistry**

**30L**

**Foundation of Quantum Mechanics**

Beginning of Quantum Mechanics: Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (without proof)

Wave function: Schrodinger time-independent equation; nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function

Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear operators; Commutation of operators, commutator and uncertainty relation; Expectation value; Hermitian operator; Postulates of Quantum Mechanics

Particle in a box: Setting up of Schrodinger equation for one-dimensional box and its solution; Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution); Expectation values of  $x$ ,  $x^2$ ,  $p_x$  and  $p_x^2$  and their significance in relation to the uncertainty principle; Extension of the problem to two and three dimensions and the concept of degenerate energy levels

Simple Harmonic Oscillator: setting up of the Schrodinger stationary equation, energy expression (without derivation), expression of wave function for  $n = 0$  and  $n = 1$  (without derivation) and their characteristic features

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)

#### **Suggested Readings:**

1. Castellan, G. W. *Physical Chemistry*, Narosa
2. Atkins, P. W. & Paula, J. de *Atkins', Physical Chemistry*, Oxford University Press
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
5. Moore, W. J. *Physical Chemistry*, Orient Longman
6. Mortimer, R. G. *Physical Chemistry*, Elsevier
7. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
8. Levine, I. N. *Quantum Chemistry*, PHI
9. Atkins, P. W. *Molecular Quantum Mechanics*, Oxford
10. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
11. Maron, S.H., Prutton, C. F., *Principles of Physical Chemistry*, McMillan
12. Klotz, I.M., Rosenberg, R. M. *Chemical Thermodynamics: Basic Concepts and Methods* Wiley
13. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
14. Glasstone, S. *An Introduction to Electrochemistry*, East-West Press

#### **CC8P : Lab-Physical Practical III:**

**45L**

**Course objectives and expected outcome:** The course provides training in advanced physical chemistry laboratory techniques. The experiments are guided by demonstrators and are designed both to illustrate the applications of theory covered in the Chemical Physics and lecture courses, and to introduce typical instrumentation. On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.

2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.
8. Developed skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
9. Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

Experiment 1: Determination of solubility of sparingly soluble salt in water, in electrolyte with common ions and in neutral electrolyte (using common indicator)

Experiment 2: Potentiometric titration of Mohr's salt solution against standard  $K_2Cr_2O_7$  solution

Experiment 3: Determination of  $K_{sp}$  for AgCl by potentiometric titration of  $AgNO_3$  solution against standard KCl solution

Experiment 4: Effect of ionic strength on the rate of Persulphate – Iodide reaction

Experiment 5: Study of phenol-water phase diagram

Experiment 6: pH-metric titration of acid (mono- and di-basic) against strong base

#### **Suggested Readings:**

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.

### **Core Course-9 (Credits: Theory-04, Practicals-02)**

#### **CC9T:INORGANIC CHEMISTRY-IV 60L**

**Course objectives and expected outcome:** Facilitate the learner to understand about coordination chemistry, transition metals, and color complex.

#### **Unit-I: Coordination Chemistry-II 25L**

VB description and its limitations. Elementary Crystal Field Theory: splitting of  $d_n$  configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy (CFSE) in weak and strong fields; pairing energy. Spectrochemical series. Jahn-Teller distortion. Octahedral site stabilization energy (OSSE). Metal-ligand bonding (MO concept, elementary idea), sigma- and pi-bonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals (examples). Magnetism and Colour: Orbital and spin magnetic moments, spin only moments of  $d_n$  ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and

antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for 3d<sup>1</sup> to 3d<sup>9</sup> ions. Racah parameter. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

**Unit-II: 30L**

### **Chemistry of d- and f- block elements**

#### **Transition Elements:**

General comparison of 3d, 4d and 5d elements in term of electronic configuration, oxidation states, redox properties, coordination chemistry.

#### **Lanthanoids and Actinoids:**

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

#### **Reference Books**

1. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
2. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann. 1997.
3. Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., Advanced Inorganic Chemistry 6th Ed. 1999., Wiley.
4. Atkin, P. Shriver & Atkins <sup>7</sup> Inorganic Chemistry 5th Ed. Oxford University Press (2010).
5. Purecell, K.F. and Kotz, J.C., An Introduction to Inorganic Chemistry, Saunders: Philadelphia, 1980.
6. Sinha, S. P., Ed., Lanthanide and Actinide Research (Journal, Vol. 1, 1986).
7. Wulfsberg, G., Principles of Descriptive Inorganic Chemistry, Brooks/Cole: Monterey, CA, 1987.

### **CC9P: Inorganic Chemistry-IV Lab**

**45L**

**Course objectives and expected outcome:** Facilitate the learner to understand about iodometric titration and estimation

#### **Iodo-/ Iodimetric Titrations**

1. Estimation of Cu(II)

2. Estimation of Vitamin C
3. Estimation of (i) arsenite and (ii) antimony in tartar-emeti iodimetrically
4. Estimation of available chlorine in bleaching powder.

#### **Estimation of metal content in some selective samples**

1. Estimation of Cu in brass.
2. Estimation of Cr and Mn in Steel.
3. Estimation of Fe in cement.

#### **Suggested Readings :**

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

#### **Core Course : 10 Credit: 06 (Theoretical:04;Practical:02)**

#### **CC-10: Organic Chemistry-III**

#### **CC10T: Organic Chemistry-III**

**Credits 04 60L**

**Course objectives and expected outcome:** Facilitate the learner to understand about substitution reactions in aliphatic as well as aromatic compounds,. They will know about about carbonyl and related compounds, organometallics and will gain knowledge about Elementary ideas of Green Chemistry.

#### **Unit-I: 20L**

#### **Substitution Reactions**

*Free-radical substitution reaction:* halogenation of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.

*Nucleophilic substitution reactions:* substitution at  $sp^3$  centre: mechanisms (with evidence), relative rates & stereochemical features:  $S_N1$ ,  $S_N2$ ,  $S_N2'$ ,  $S_N1'$  (allylic rearrangement) and  $S_Ni$ ; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP; role of crown ethers and phase transfer catalysts; [systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides].

#### **Aromatic Substitution**

*Electrophilic aromatic substitution:* mechanisms and evidences in favour of it; orientation and reactivity; reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reaction; one-carbon electrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Houben-Hoesch, Vilsmeier-Haack, Reimer-Tiemann, Kolbe-Schmidt); *Ips*o substitution.

*Nucleophilic aromatic substitution:* addition-elimination mechanism and evidences in favour of it;  $S_N1$  mechanism; cine substitution (benzyne mechanism), structure of benzyne.

#### **Unit-II: 20L**

#### **Carbonyl and Related Compounds**

*Addition to C=O:* structure, reactivity and preparation of carbonyl compounds; mechanism (with evidence), reactivity, equilibrium and kinetic control; Burgi-Dunitz trajectory in nucleophilic additions; formation of hydrates, cyano hydrins and bisulphite adduct; nucleophilic addition-elimination reactions with alcohols, thiols and nitrogen- based nucleophiles; reactions: benzoin condensation, Cannizzaro and Tischenko reactions, reactions with ylides: Wittig and Corey-Chaykovsky reaction; Rupe rearrangement, oxidations and reductions: Clemmensen, Wolff-Kishner,  $LiAlH_4$ ,  $NaBH_4$ , MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.

*Exploitation of acidity of  $\alpha$ -H of C=O:* formation of enols and enolates; kinetic and thermodynamic enolates; reactions (mechanism with evidence): halogenation of carbonyl compounds under acidic and basic conditions, Hell-Volhard-Zelinsky (H. V. Z.) reaction, nitrosation,  $SeO_2$  (Riley) oxidation;

condensations (mechanism with evidence): Aldol, Tollens', Knoevenagel, Claisen-Schmidt, Claisen ester including Dieckmann, Stobbe; Mannich reaction, Perkin reaction, Favorskii rearrangement; alkylation of active methylene compounds; preparation and synthetic applications of diethyl malonate and ethyl acetoacetate; specific enol equivalents (lithium enolates, enamines, aza-enolates and silyl enol ethers) in connection with alkylation, acylation and aldol type reaction.

*Nucleophilic addition to  $\alpha,\beta$ -unsaturated carbonyl system:* general principle and mechanism (with evidence); direct and conjugate addition, addition of enolates (Michael reaction), Stetter reaction, Robinson annulation.

**Substitution at  $sp^2$  carbon (C=O system):** mechanism (with evidence):  $B_{AC2}$ ,  $A_{AC2}$ ,  $A_{AC1}$ ,  $A_{AL1}$  (in connection to acid and ester); acid derivatives: amides, anhydrides & acyl halides (formation and hydrolysis including comparison).

### Unit-III: 20L Organometallics

*Grignard reagent; Organolithiums; Gilman cuprates:* preparation and reactions (mechanism with evidence); addition of Grignard and organolithium to carbonyl compounds; substitution on -COX; directed ortho metalation of arenes using organolithiums, conjugate addition by Gilman cuprates; Corey-House synthesis; abnormal behavior of Grignard reagents; comparison of reactivity among Grignard, organolithiums and organocopper reagents; Reformatsky reaction; Blaise reaction; concept of *umpolung* and base-nucleophile dichotomy in case of organometallic reagents.

**Elementary ideas of Green Chemistry:** Twelve (12) principles of green chemistry; planning of green synthesis; common organic reactions and their counterparts: reactions: Aldol, Friedel-Crafts, Michael, Knoevenagel, Cannizzaro, benzoin condensation and Dieckmann condensation.

### Suggested Readings:

1. Clayden, J., Greeves, N., Warren, S. *Organic Chemistry*, Second edition, Oxford University Press 2012.
2. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
3. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
4. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
5. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press, 2008.
6. Norman, R.O. C., Coxon, J. M. *Principles of Organic Synthesis*, Third Edition, Nelson Thornes, 2003.
7. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
8. Finar, I. L. *Organic Chemistry (Volume 1)*, Pearson Education.
9. Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry*, John Wiley & Sons, Inc.
10. March, J. *Advanced Organic Chemistry*, Fourth edition, Wiley.
11. Jenkins, P. R., *Organometallic Reagents in Synthesis*, Oxford Chemistry Primer, Oxford University Press.
12. Ward, R. S., *Bifunctional Compounds*, Oxford Chemistry Primer, Oxford University Press.
13. Ahluwalia, V. K. *Strategies for Green Organic Synthesis*, ANE Books Pvt. Ltd.

**Course objectives and expected outcome:** Facilitate the learner to understand about Qualitative Analysis of Single Solid Organic Compounds.

### Experiment -1: Qualitative Analysis of Single Solid Organic Compounds

- Detection of special elements (N, S, Cl, Br) by Lassaigne's test
- Solubility and classification (solvents: H<sub>2</sub>O, 5% HCl, 5% NaOH and 5% NaHCO<sub>3</sub>)
- Detection of the following functional groups by systematic chemical tests: aromatic amino (-NH<sub>2</sub>), aromatic nitro (-NO<sub>2</sub>), amido (-CONH<sub>2</sub>, including imide), phenolic -OH, carboxylic acid (-COOH), carbonyl (-CHO and >C=O); only one test for each functional group is to be reported.
- Melting point of the given compound
- Preparation, purification and melting point determination of a crystalline derivative of the given compound
- Identification of the compound through literature survey.

Each student, during laboratory session, is required to carry out qualitative chemical tests for all the special elements and the functional groups with relevant derivatisation in known and unknown (**at least six**) organic compounds.

### Suggested Readings:

- Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.
- University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N. University of Calcutta, 2003.
- 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).
- Clarke, H. T., *A Handbook of Organic Analysis (Qualitative and Quantitative)*, Fourth Edition, CBS Publishers and Distributors (2007).
- Practical Workbook Chemistry (Honours), UGBS, Chemistry*, University of Calcutta, 2015.

## Skill Enhancement Course (SEC)

### SEC-II (Credit:2) Any one of the following

- SEC: CHEMISTRY OF COSMETICS & PERFUMES** Credit 02

**SEC-T: CHEMISTRY OF COSMETICS & PERFUMES      15L Credit 01**

**Course objectives and expected outcome:** Facilitate the learner to understand about the preparation of cosmetic products and some essential oils.

**Course Contents:**

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

**SEC-P: Practicals      15L****Credits 01**

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

**Suggested Readings:**

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

**2. SEC: PESTICIDE CHEMISTRY****Credit 02****SEC-T: PESTICIDE CHEMISTRY      15L      Credit 01**

**Course objectives and expected outcome:** Facilitate the learner to understand about natural and synthetic pesticides ,their benefits and adverse effects , technical manufacture and uses of representative pesticides.

**Course Contents:**

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion ); Carbamates (Carbofuran and carbaryl); Quinones ( Chloranil), Anilides (Alachlor and Butachlor).

**SEC-P: Practicals****Credit 01**

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

**Suggested Readings:**

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

**3. SEC: FUEL CHEMISTRY      30L****Credits 02****SEC-T: FUEL CHEMISTRY**

**Course objectives and expected outcome:** Facilitate the learner to Review of energy sources



(renewable and non-renewable), Petroleum and Petrochemical Industry, Petrochemicals, Lubricants.

**Course Contents:**

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

**Suggested Readings:**

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

**4. SEC: INTELLECTUAL PROPERTY RIGHTS (IPR) (Credits: 02)**

**Theory: 30L**

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

**Introduction to Intellectual Property:**

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

**Copyrights**

Introduction, How to obtain, Differences from Patents.

**Trade Marks**

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

Differences from Designs.

**Patents**

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

### **Geographical Indications**

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

### **Industrial Designs**

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

### **Layout design of integrated circuits**

Circuit Boards, Integrated Chips, Importance for electronic industry.

### **Trade Secrets**

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

### **Different International agreements**

#### **(a) World Trade Organization (WTO):**

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

#### **(b) Paris Convention**

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

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

### **Reference Books:**

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

**Core Course-11: Credit: 06 (Theoretical: 04; Practical: 02)**

## **Physical Chemistry-IV**

**CC11T: Physical Chemistry-IV 60L**

**Course objectives and expected outcome:** From this section students will gain knowledge about interaction of electromagnetic radiation with molecules and various types of spectra, Rotation spectroscopy, Vibrational spectroscopy, Raman spectroscopy, Nuclear Magnetic Resonance (NMR) spectroscopy, Electron Spin Resonance (ESR) spectroscopy, photochemistry, solid state and Surface phenomenon. This topic facilitates to detect, determine, or quantify the molecular and/or structural composition of a sample.

### **Unit-I: Molecular Spectroscopy 25L**

1. Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation
2. **Rotation spectroscopy:** Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution
3. **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; Diatomic vibrating rotator, P, Q, R branches
4. **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
5. **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
6. **Electron Spin Resonance (ESR) spectroscopy:** Its principle, hyperfine structure, ESR of simple radicals

### **Unit-II: Photochemistry 15L**

1. Lambert-Beer's law: Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients; Laws of photochemistry, Stark-Einstein law of photochemical equivalence quantum yield, actinometry, examples of low and high quantum yields

2. Photochemical Processes: Potential energy curves (diatomic molecules), Frank-Condon principle and vibrational structure of electronic spectra; Bond dissociation and principle of determination of dissociation energy (ground state); Decay of excited states by radiative and non-radiative paths; Pre-dissociation; Fluorescence and phosphorescence, Jablonskii diagram;

3. Rate of Photochemical processes: Photochemical equilibrium and the differential rate of photochemical reactions, Photostationary state; HI decomposition, H<sub>2</sub>-Br<sub>2</sub> reaction, dimerisation of anthracene; photosensitised reactions, quenching; Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence

### **Unit:III- Surface phenomenon 20L**

1. Surface tension and energy: Surface tension, surface energy, excess pressure, capillary rise and surface tension; Work of cohesion and adhesion, spreading of liquid over other surface; Vapour pressure over curved surface; Temperature dependence of surface tension

2. Adsorption: Physical and chemical adsorption; Freundlich and Langmuir adsorption isotherms; multilayer adsorption and BET isotherm (no derivation required); Gibbs adsorption isotherm and surface excess; Heterogenous catalysis (single reactant); Zero order and fractional order reactions;

3. Colloids: Lyophobic and lyophilic sols, Origin of charge and stability of lyophobic colloids, Coagulation and Schultz-Hardy rule, Zeta potential and Stern double layer (qualitative idea), Tyndall effect; Electrokinetic phenomena (qualitative idea only); Determination of Avogadro number by Perrin's method; Stability of colloids and zeta potential; Micelle formation.

### **Crystalline State**

Laws of Crystallography, unit cell, lattice, different crystalline systems with characteristics, Bragg's equation, application towards structure of NaCl and KCl. Specific heats of solid elements, Dulong-Petit's law, limitations, Einstein's equation, success and limitations, Debye's  $T^3$  law (no derivation)

### **Reference Books**

1. Castellan, G. W. Physical Chemistry, Narosa
2. Levine, I. N. Physical Chemistry, Tata McGraw-Hill
3. Atkins, P. W. & Paula, J. de Atkin's, Physical Chemistry, Oxford University Press

4. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
5. Mortimer, R. G. Physical Chemistry, Elsevier Laidler, K. J. Chemical Kinetics, Pearson
6. Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill
7. Barrow, G. M. Molecular Spectroscopy, McGraw-Hill Hollas, J.M. Modern Spectroscopy, Wiley India
8. McHale, J. L. Molecular Spectroscopy, Pearson Education
9. Wayne, C. E. & Wayne, R. P. Photochemistry, OUP
10. Brown, J. M. Molecular Spectroscopy, OUP
11. Levine, I. N. Quantum Chemistry, PHI
12. Atkins, P. W. Molecular Quantum Mechanics, Oxford

#### **CC11P : Lab-Physical Practical IV: 45L**

**Course objectives and expected outcome:** The course provides training in advanced physical chemistry laboratory techniques. The experiments are guided by demonstrators and are designed both to illustrate the applications of theory covered in the Chemical Physics and lecture courses, and to introduce typical instrumentation. On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.
2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.
8. Developed skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
9. Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

1. Determination of surface tension of a liquid using Stalagmometer
2. Determination of CMC from surface tension measurements
3. Verification of Beer and Lambert's Law for  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  solution
4. Study of kinetics of  $\text{K}_2\text{S}_2\text{O}_8 + \text{KI}$  reaction, spectrophotometrically
5. Determination of pH of unknown buffer, spectrophotometrically
6. Spectrophotometric determination of CMC

#### **Reference Books**

Viswanathan, B., Raghavan, P.S. Practical Physical Chemistry Viva Books (2009) Mendham,

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

Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007)

Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency

University Hand Book of Undergraduate Chemistry Experiments, edited by  
Mukherjee, G. N., University of Calcutta

Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd. Gurtu, J.

N., Kapoor, R., Advanced Experimental Chemistry S. Chand & Co. Ltd.

## **Core Course : 12 Credit: 06 (Theoretical:04;Practical:02)**

### **CC-12: ORGANIC CHEMISTRY-IV**

#### **CC12T: ORGANIC CHEMISTRY-IV 60L**

**Credits 04**

**Course objectives and expected outcome:** They will gain the knowledge about the synthesis, properties, spectroscopic characterization and utilities of carbon oxygen, Nitrogen containing organic compounds which are essential to our daily life.

#### **Unit:-I - Nitrogen compounds 15L**

*Amines: Aliphatic & Aromatic:* preparation, separation (Hinsberg's method) and identification of primary, secondary and tertiary amines; reaction (with mechanism): Eschweiler-Clarke methylation, diazo coupling reaction, Mannich reaction; formation and reactions of phenylenediamines, diazomethane and diazoacetic ester.

*Nitro compounds (aliphatic and aromatic):* preparation and reaction (with mechanism): reduction under different conditions; Nef carbonyl synthesis, Henry reaction and conjugate addition of nitroalkane anion.

*Alkyl nitrile and isonitrile:* preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.

*Diazonium salts and their related compounds:* reactions (with mechanism) involving replacement of diazo group; reactions: Gomberg, Meerwein, Japp-Klingermann.

#### **Unit:-II- Rearrangements 15L**

*Mechanism with evidence and stereochemical features for the following*

*Rearrangement to electron-deficient carbon:* Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzil-benzilic acid rearrangement, Demjanov rearrangement, Tiffeneau-Demjanov rearrangement.

*Rearrangement to electron-deficient nitrogen:* rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann.

*Rearrangement to electron-deficient oxygen:* Baeyer-Villiger oxidation, cumene hydroperoxide-

phenol rearrangement and Dakin reaction.

*Aromatic rearrangements: Migration from oxygen to ring carbon:* Fries rearrangement and Claisen rearrangement.

*Migration from nitrogen to ring carbon:* Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, *N*-azo to *C*-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.

*Rearrangement reactions by green approach:* Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

### **Unit-III:- The Logic of Organic Synthesis 10L**

*Retrosynthetic analysis:* disconnections; synthons, donor and acceptor synthons; natural reactivity and *umpolung*; latent polarity in bifunctional compounds: consonant and dissonant polarity; illogical electrophiles and nucleophiles; synthetic equivalents; functional group interconversion and addition (FGI and FGA); C-C disconnections and synthesis: one-group and two-group (1,2- to 1,5-dioxygenated compounds), reconnection (1,6-dicarbonyl); protection-deprotection strategy (alcohol, amine, carbonyl, acid).

*Strategy of ring synthesis:* thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.

*Asymmetric synthesis:* stereoselective and stereospecific reactions; diastereoselectivity and enantioselectivity (only definition); enantioselectivity: kinetically controlled MPV reduction; diastereoselectivity: addition of nucleophiles to C=O adjacent to a stereogenic centre: Felkin-Anh and Zimmermann-Traxler models.

### **Unit:- IV- Organic Spectroscopy 20L**

*UV Spectroscopy:* introduction; types of electronic transitions, end absorption; transition dipole moment and allowed/forbidden transitions; chromophores and auxochromes; Bathochromic and Hypsochromic shifts; intensity of absorptions (Hyper-/Hypochromic effects); application of Woodward's Rules for calculation of  $\lambda_{\max}$  for the following systems: conjugated diene,  $\alpha,\beta$ -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of  $\lambda_{\max}$  considering conjugative effect, steric effect, solvent effect, effect of pH; effective chromophore concentration: keto-enol systems; benzenoid transitions.

*IR Spectroscopy:* introduction; modes of molecular vibrations (fundamental and non-fundamental); IR active molecules; application of Hooke's law, force constant; fingerprint region and its significance; effect of deuteration; overtone bands; vibrational coupling in IR; characteristic and diagnostic stretching frequencies of C-H, N-H, O-H, C-O, C-N, C-X, C=C (including skeletal vibrations of aromatic compounds), C=O, C=N, N=O, C $\equiv$ C, C $\equiv$ N; characteristic/diagnostic bending vibrations are included; factors affecting stretching frequencies: effect of conjugation, electronic effects, mass effect, bond multiplicity, ring-size, solvent effect, H-bonding on IR absorptions; application in functional group analysis.

*NMR Spectroscopy:* introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of *first-order* multiplets: Pascal's triangle; chemical and magnetic equivalence in NMR; elementary idea about *non-first-order* splitting; anisotropic effects in alkene, alkyne, aldehydes and aromatics; NMR peak area, integration;

relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic); rapid proton exchange; interpretation of NMR spectra of simple compounds. Applications of IR, UV and NMR spectroscopy for identification of simple organic molecules.

### Suggested Readings:

1. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Norman, R.O. C., Coxon, J. M. *Principles of Organic Synthesis*, Third Edition, Nelson Thornes, 2003.
4. Clayden, J., Greeves, N., Warren, S., *Organic Chemistry*, Second edition, Oxford University Press 2012.
5. Silverstein, R. M., Bassler, G. C., Morrill, T. C. *Spectrometric Identification of Organic Compounds*, John Wiley and Sons, INC, Fifth edition.
6. Kemp, W. *Organic Spectroscopy*, Palgrave.
7. Pavia, D. L. *et al. Introduction to Spectroscopy*, 5th Ed. Cengage Learning India Ed. (2015).
8. Dyer, J. *Application of Absorption Spectroscopy of Organic Compounds*, PHI Private Limited
9. March, J. *Advanced Organic Chemistry*, Fourth edition, Wiley.
10. Harwood, L. M., *Polar Rearrangements*, Oxford Chemistry Primer, Oxford University Press.
11. Bailey, Morgan, *Organonitrogen Chemistry*, Oxford Chemistry Primer, Oxford University Press.
12. Ahluwalia, V. K. *Strategies for Green Organic Synthesis*, ANE Books Pvt. Ltd.
13. Warren, S. *Organic Synthesis the Disconnection Approach*, John Wiley and Sons.
14. Warren, S., *Designing Organic Synthesis*, Wiley India, 2009.
15. Carruthers, W. *Modern methods of Organic Synthesis*, Cambridge University Press.
16. Willis, C. A., Wills, M., *Organic Synthesis*, Oxford Chemistry Primer, Oxford University Press.

CC12P : LAB 45L

Credits 02

### Course objectives and expected outcome:

Acquire the knowledge about the quantitative estimation of different natural and artificial organic compounds.

#### List of Practical

#### Quantitative

#### Estimations:



Each student is required to perform all the experiments.

1. Estimation of glycine by Sørensen's formol method
2. Estimation of glucose by titration using Fehling's solution
3. Estimation of sucrose by titration using Fehling's solution
4. Estimation of vitamin-C (reduced)
5. Estimation of aromatic amine (aniline) by bromination (Bromate-Bromide) method
6. Estimation of phenol by bromination (Bromate-Bromide) method
7. Estimation of formaldehyde (Formalin)
8. Estimation of acetic acid in commercial vinegar
9. Estimation of urea (hypobromite method)
10. Estimation of saponification value of oil/fat/ester

**Suggested Readings:**

1. Arthur, I. V. *Quantitative Organic Analysis*, Pearson
2. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta

## Discipline Specific Elective Course (DSE-I and DSE-II)

**Any two** of the following (Total Credit:  $2*6=12$ )

### **1. CHEMISTRY-DSE: APPLICATIONS OF COMPUTERS IN CHEMISTRY**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60L**

## Course objectives and expected outcome:

Acquire the knowledge about the idea of numerical of different Computer languages and computational understanding and molecular modeling.

### Basics:

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

### Numerical methods:

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

*Differential calculus:* Numerical differentiation.

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

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

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

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

### Reference

#### Books:

- Harris, D. C. *Quantitative Chemical Analysis*. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

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## PRACTICAL-DSE      LAB: 45L

### Application of computer in chemistry

#### Course objectives and expected outcome:

Acquire the knowledge about the idea of Computer languages (C++, Fortran, Scilab) of different physio chemical reaction and computational understanding in molecular

## visualization.

Computer programs based on numerical methods for

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

## Reference

### Books:

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

## 2. CHEMISTRY-DSE: ANALYTICAL METHODS IN CHEMISTRY (Credits: Theory-04, Practicals-02)

### Theory: 60L

#### Course objectives and expected outcome:

Acquire the knowledge about the idea of spectroscopic molecular structure determination, thermogravimetry and electrochemical analysis, qualitative and quantitative extraction and separation of molecules from chromatographic analysis.

#### Qualitative and quantitative aspects of analysis:

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

and t test, rejection of data, and confidence intervals.

**Optical methods of analysis:**

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

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

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

*Infrared Spectrometry:* Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques. Structural illustration through interpretation of data, Effect and importance of isotope substitution.

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

**Thermal methods of analysis:**

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

**Electroanalytical methods:**

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

**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.

#### **Reference Books:**

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

## **PRACTICALS- DSE LAB: 45L**

### **ANALYTICAL METHODS IN CHEMISTRY**

#### **Course objectives and expected outcome:**

Hands on training about the chromatographic separation metal extraction, ion exchange soil analysis, spectroscopic oxygen demand calculation.

#### **I. Separation Techniques**

##### **1. Chromatography:**

(a) Separation of mixtures

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

(ii) Separation and identification of the monosaccharides present in the given mixture

(glucose & fructose) by paper chromatography. Reporting the  $R_f$  values.

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

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

## II. Solvent

### Extractions:

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

(ii) Solvent extraction of zirconium 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 flame photometric techniques.

### 5. Analysis of soil:

(i) Determination of pH of

soil. (ii) Total soluble salt

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

### 6. Ion exchange:

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins. (ii) Separation of metal ions from their binary mixture.

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

## III Spectrophotometry

1. Determination of pK<sub>a</sub> values of indicator using spectrophotometry.

2 Structural characterization of compounds by infrared spectroscopy.

3 Determination of dissolved oxygen in water.

4 Determination of chemical oxygen demand (COD).

5 Determination of Biological oxygen demand (BOD).

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

### Reference Books:

- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5<sup>th</sup> Ed. The English Language Book Society of Longman .
- Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7<sup>th</sup> Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman,

2001.

- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
  - Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
  - Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
  - Ditts, R.V. Analytical Chemistry – Methods of separation.
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### **3. CHEMISTRY-DSE: MOLECULAR MODELLING & DRUG DESIGN (Credits: Theory-04, Practicals-02)**

#### **Theory: 60L**

##### **Course objectives and expected outcome:**

Theoretical training about the molecular modeling, simulation of energy minimization, molecular dynamics, drug designing and preliminary knowledge about chemo informatics.

##### **Introduction to Molecular Modelling:**

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

##### **Force Fields:**

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

##### **Energy Minimization and Computer Simulation:**

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

##### **Molecular Dynamics & Monte Carlo Simulation:**

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

## Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative 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.

## Reference Books:

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

## PRACTICAL- DSE LAB: 45L

### Course objectives and expected outcome:

Computational training about the optimization of bond length, bond energy conformational and configurational analysis, visualization of electrostatic potential map, comparison of boiling point of different organic molecules, optimization of bond angle and above all learning of various software like chemsketch, Arguslab, Tinker.

## MOLECULA MODELLING & DRUG DESIGN

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene.  
  
Visualize the molecular orbitals of the ethane  $\sigma$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  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<sub>2</sub>, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118°C, 100°C, 108°C, 82°C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-



methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

- ix. (a) Compare the optimized bond angles  $\text{H}_2\text{O}$ ,  $\text{H}_2\text{S}$ ,  $\text{H}_2\text{Se}$ . (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](http://www.planaria-software.com)), TINKER ([dasher.wustl.edu/ffe](http://dasher.wustl.edu/ffe)), WebLab Viewer, Hyperchem, or any similar software.

#### Reference Books:

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

#### 4. CHEMISTRY-DSE: POLYMER CHEMISTRY (Credits: Theory-06, Practicals-02)

##### Theory: 60L

##### Course objectives and expected outcome:

Since ancient times, polymers have been part of our natural world. Current applications extend from adhesives, coatings, foams, and packaging materials to textile and industrial fibers, composites, electronic devices, biomedical devices, optical devices, and precursors for many newly developed high-tech ceramics. The list is almost endless. These manifold uses of polymers have immensely helped to raise our living standards. Effect of temperature on polymerization, kinetics & mechanism. Kinetics and utility of copolymerization reaction. Evaluate the effect of reactivity ratio of monomers on the type of copolymer and copolymer composition to produce a copolymer of desired properties. Melting point also known as melt temperature is the critical temperature above which the crystalline regions in a semicrystalline plastic are able to flow. Rationalize bulk properties and processes using thermodynamic considerations. Electrochemical properties of polymers.

##### Introduction and history of polymeric materials:

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

##### Functionality and its importance:

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

##### Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and

anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

### **Crystallization and crystallinity:**

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

**Nature and structure of polymers**-Structure Property relationships.

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

Polydispersity index.

**Glass transition temperature (T<sub>g</sub>) and determination of T<sub>g</sub>**, Free volume theory, WLF equation, Factors affecting glass transition temperature (T<sub>g</sub>).

**Polymer Solution** – Criteria for polymer solubility, Solubility parameter,

Thermodynamics

of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

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

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

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

### **Reference**

#### **Books:**

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

## **CHEMISTRY PRACTICAL - DSE LAB: 45L**

### **POLYMER CHEMISTRY**

**Course objectives and expected outcome:** The course provides training in advanced physical chemistry laboratory techniques. The experiments are guided by demonstrators and are designed both to illustrate the applications of theory covered in the Chemical Physics and lecture courses, and to introduce typical instrumentation. On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.
2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.
8. Developed skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
9. Developed some understanding of the professional and safety responsibilities residing in working with chemical systems.

#### **1. Polymer synthesis**

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

#### **Polymer characterization**

1. Determination of molecular weight by viscometry: (a) Polyacrylamide-aq.NaNO<sub>2</sub> solution (b) (Poly vinyl propylidene (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol)

(PVOH) and the fraction of “head-to-head” monomer linkages in the polymer.

3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

#### **Polymer analysis**

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. IR studies of polymers
4. DSC analysis of polymers
5. Preparation of polyacrylamide and its electrophoresis

\*at least 7 experiments to be carried out.

#### **Reference Books:**

- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3<sup>rd</sup> Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3<sup>rd</sup> ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3<sup>rd</sup> ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2<sup>nd</sup> ed. Prentice-Hall (2003)
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2<sup>nd</sup> ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4<sup>th</sup> ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3<sup>rd</sup> ed. Oxford University Press (2005)
- Seymour/ Carraher’s Polymer Chemistry, 9<sup>th</sup> ed. by Charles E. Carraher, Jr. (2013).

## **Theory: 60L**

### **Course objectives and expected outcome:**

Students learn about energy and environmental studies, energy resources, industrial gases, manufacture of hazardous inorganic materials, pollutions (air, water) and controlling process, biogeochemical cycles, biocatalyst synthesis and their applications to society.

### **Industrial Gases and Inorganic Chemicals**

*Industrial Gases:* Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene. *Inorganic Chemicals:* Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

### **Industrial Metallurgy**

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

### **Environment and its segments**

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

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

Pollution by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases. Methods of estimation of CO, NO<sub>x</sub>, SO<sub>x</sub> and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates

*Water Pollution:* Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

### **Energy & Environment**

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy,

Hydrogen, geothermal, Tidal and Hydel, etc.

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

### **Biocatalysis**

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

### **Reference Books:**

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- J. A. Kent: *Riegel’s Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
- K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
- S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
- S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
- G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
- A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).

## **CHEMISTRY PRACTICAL - DSE LAB: 45L**

### **Course objectives and expected outcome:**

Students get practical knowledge to acquire oxygen demined, quantitative chlorine estimation, estimation of total alkalinity of water samples and preparation of borax and boric acid.

## **INDUSTRIAL CHEMICALS & ENVIRONMENT**

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 ( $\text{AgNO}_3$  and potassium chromate).
6. Estimation of total alkalinity of water samples ( $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ) using double titration method.

7. Measurement of dissolved CO<sub>2</sub>.
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

#### Reference Books:

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

### Core Course -13 (Credits: Theory-04, Practicals-02)

#### CC13T: INORGANIC CHEMISTRY-V 60L

#### Course objectives and expected outcome:

Students get theoretical knowledge about the role of metal to biological system, metal-carbon bond formation and their stability, Complex metric reaction kinetics and mechanism.

#### Unit-I: Bioinorganic Chemistry 15L

Elements of life: essential and beneficial elements, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, Fe<sup>3+/2+</sup>, Cu<sup>2+/+</sup>, and Zn<sup>2+</sup>). Metal ion transport across biological membrane Na<sup>+</sup>/ K<sup>+</sup> ion pump. Dioxygen molecule in life. Dioxygen management proteins: Haemoglobin, Myoglobin, Hemocyanine and Hemerythrin. Electron transfer proteins: Cytochromes and Ferredoxins. Hydrlytic enzymes: carbonate bicarbonate buffering system and carbonic anhydrase and carboxyanhydrase A. Biological nitrogen fixation, Photosynthesis: Photosystem-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases (examples only)

## **Unit-II- Organometallic Chemistry 15L**

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. 18-electron and 16-electron rules (pictorial MO approach). Applications of 18-electron rule to metal carbonyls, nitrosyls, cyanides. General methods of preparation of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls. pi-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation, structure, evidences of synergic effect. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination and insertion reactions.

## **Unit-III: Catalysis by Organometallic Compounds 15L**

Study of the following industrial processes

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Hydroformylation
3. Wacker Process
4. Synthetic gasoline (Fischer Tropsch reaction)
5. Ziegler-Natta catalysis for olefin polymerization.

## **Unit-IV: Reaction Kinetics and Mechanism 15L**

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect and its application in complex synthesis, 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.

### **Reference Books**

1. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
2. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
3. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
4. Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., Advanced Inorganic Chemistry 6th Ed. 1999., Wiley.
5. Bertini, I., Gray, H. B., Lippard, S.J., Valentine, J. S., Viva, 2007.
6. Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.



7. Purecell, K.F. and Kotz, J.C., An Introduction to Inorganic Chemistry, Saunders: Philadelphia, 1980.
8. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
9. Collman, J. P. et al. Principles and Applications of Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
10. Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000.

### **CC13P: Inorganic Chemistry-IV –Lab 45L**

#### **Course objectives and expected outcome:**

Students get hands on training about the chromatographic separation of metal ions and spectrophotometric estimation.

#### **Chromatography of metal ions**

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

1. Ni (II) and Co (II)
2. Fe (III) and Al (III)

#### **Gravimetry**

1. Estimation of nickel (II) using Dimethylglyoxime (DMG).
2. Estimation of copper as CuSCN
3. Estimation of Al (III) by precipitating with oxine and weighing as Al(oxine)<sub>3</sub> (aluminium oxinate)
4. Estimation of chloride

#### **Spectrophotometry**

1. Measurement of 10Dq by Spectrophotometric method
2. Determination of Max of [Mn(acac)<sub>3</sub>] and [Fe(acac)<sub>3</sub>] complexes

#### **Reference Books**

Mendham, J., A. I. Vogel's Quantitative Chemical

**Core Course 14: Credit 6 (Theoretical: 4 & Practical:2)**

**CC14T - Organic Chemistry V 60L**

## Organic Chemistry V (Theory)

4 Credit

### Course objectives and expected outcome:

- Acquire knowledge about synthesis and common chemical reaction of carbocyclic molecules (naphthalene, anthracene, phenanthrene) and heterocyclic molecules (pyrrole, furan, thiophene, pyridine).
- Brief knowledge about a few chemical reactions and stereochemistry of alicyclic molecules.
- Gather brief knowledge about various pericyclic reactions and their FMO approach.
- Some basic understanding of structure of different bio-molecules like carbohydrate, peptide, nucleic acid and their reactions.
- Brief introduction about organic dyes, structure and their classification.

### Unit-I: Carbocycles and Heterocycles 10L

1. Polynuclear hydrocarbons and their derivatives: synthetic methods include Haworth, Bardhan-Sengupta, Bogert-Cook and other useful syntheses (with mechanistic details); fixation of double bonds and Fries rule; reactions (with mechanism) of naphthalene, anthracene, phenanthrene and their derivatives.
2. Heterocyclic compounds: 5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole, thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist-Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis; benzo-fused 5- and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approach and mechanistic details): indole: Fischer, Madelung and Reissert; quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: Bischler-Napieralski synthesis.

### Unit-II: Cyclic Stereochemistry 10L

Alicyclic compounds: concept of I-strain; conformational analysis: cyclohexane, mono and disubstituted cyclohexane; symmetry properties and optical activity; topomerisation; ring-size and ease of cyclisation; conformation & reactivity in cyclohexane system: consideration of steric and stereoelectronic requirements; elimination (E<sub>2</sub>, E<sub>1</sub>), nucleophilic substitution (S<sub>N</sub>1, S<sub>N</sub>2, S<sub>N</sub>i, N<sub>GP</sub>), merged substitution-elimination; rearrangements; oxidation of cyclohexanol, esterification, saponification, lactonisation,

epoxidation, pyrolytic syn elimination and fragmentation reactions.

### Unit-III: Pericyclic reactions 10L

Mechanism, stereochemistry, regioselectivity in case of

1. Electrocyclic reactions: FMO approach involving  $4\pi$  and  $6\pi$  electrons (thermal and photochemical) and corresponding cycloreversion reactions.
2. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions.
3. Sigmatropic reactions: FMO approach, sigmatropic shifts and their order; [1,3]- and [1,5]-H shifts and [3,3]-shifts with reference to Claisen and Cope rearrangements.

### Unit-IV: Carbohydrates 30L

1. Monosaccharides: Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms): Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine-water oxidation,  $\text{HNO}_3$  oxidation, selective oxidation of terminal  $-\text{CH}_2\text{OH}$  of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping-up (Kiliani-Fischer method) and stepping-down (Ruff's & Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene) and benzylidene protections; ring-size determination; Fischer's proof of configuration of (+)-glucose.
2. Disaccharides: Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar.
3. Polysaccharides: starch (structure and its use as an indicator in titrimetric analysis).

### Biomolecules

1. Amino acids: synthesis with mechanistic details: Strecker, Gabriel, acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine; isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.
2. Peptides: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using N-protection & C-protection, solid-phase (Merrifield) synthesis;

peptide sequence: C-terminal and N-terminal unit determination (Edman, Sanger & ‘dansyl’ methods); partial hydrolysis; specific cleavage of peptides: use of CNBr.

3. Nucleic acids: pyrimidine and purine bases (only structure & nomenclature); nucleosides and nucleotides corresponding to DNA and RNA; mechanism for acid catalysed hydrolysis of nucleosides (both pyrimidine and purine types); comparison of alkaline hydrolysis of DNA and RNA; elementary idea of double helical structure of DNA (Watson-Crick model); complimentary base-pairing in DNA.

## 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; Natural dyes — structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

## Reference Books

1. Clayden, J., Greeves, N., Warren, S. Organic Chemistry, Second edition, Oxford University Press 2012.
2. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London.
3. Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
4. Sen Gupta, Subrata. Basic Stereochemistry of Organic molecules.
5. Kalsi, P. S. Stereochemistry Conformation and Mechanism, Eighth edition, New Age International, 2014.
6. Fleming, I. Molecular Orbitals and Organic Chemical reactions, Reference/Student Edition, Wiley, 2009.
7. Fleming, I. Pericyclic Reactions, Oxford Chemistry Primer, Oxford University Press.
8. Gilchrist, T. L. & Storr, R. C. Organic Reactions and Orbital symmetry, Cambridge University Press.
9. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
10. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
11. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd.
12. Loudon, G. M. Organic Chemistry, Fourth edition, Oxford University Press.
13. James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003.

14. Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005.
15. Davis, B. G., Fairbanks, A. J., Carbohydrate Chemistry, Oxford Chemistry Primer, Oxford University Press.
16. Joule, J. A. Mills, K. Heterocyclic Chemistry, Blackwell Science.
17. Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Wiley & Sons (1976).
18. Gilchrist, T. L. Heterocyclic Chemistry, 3rd edition, Pearson.
19. Bansal, R. K. Heterocyclic Chemistry, New Age International Publishers.
20. Davies, D. T., Heterocyclic Chemistry, Oxford Chemistry Primer, Oxford University Press.

### **CC14P - Organic Chemistry V Lab**

#### **Organic Chemistry V (Lab) 45L**

**2 Credit**

#### **Course objectives and expected outcome:**

- Acquire knowledge about different chromatographic separation technique (TLC, Column, Paper) of mixture of amino acids, dyes and sugars.
- IR and NMR spectroscopic analysis of different organic groups having specific functional group.

#### **Chromatographic Separations**

1. TLC separation of a mixture containing 2/3 amino acids
2. TLC separation of a mixture of dyes (fluorescein and methylene blue)
3. Column chromatographic separation of leaf pigments from spinach leaves
4. Column chromatographic separation of mixture of dyes
5. Paper chromatographic separation of a mixture containing 2/3 amino acids
6. Paper chromatographic separation of a mixture containing 2/3 sugars

#### **Spectroscopic Analysis of Organic Compounds**

1. Assignment of labeled peaks in the  $^1\text{H-NMR}$  spectra of the known organic compounds explaining the relative  $\delta$ -values and splitting pattern.
2. Assignment of labelled peaks in the IR spectrum of the same compound explaining the relative frequencies of the absorptions (C-H, O-H, N-H, C-O, C-N, C-X, C=C, C=O, N=O, C C, C N stretching frequencies; characteristic bending vibrations are included).
3. The students must record full spectral analysis of at least 15 (fifteen) compounds from the following list:
  - a. 4-Bromoacetanilide
  - b. 2-Bromo-4'-methylacetophenone

- c. Vanillin
- d. 2-Methoxyacetophenone
- e. 4-Aminobenzoic acid
- f. Salicylamide
- g. 2-Hydroxyacetophenone
- h. 1,3-Dinitrobenzene
- i. Benzylacetate
- j. trans-4-Nitrocinnamaldehyde
- k. Diethyl fumarate
- l. 4-Nitrobenzaldehyde
- m. 4-Methylacetanilide
- n. Mesityl oxide
- o. 2-Hydroxybenzaldehyde
- p. 4-Nitroaniline
- q. 2-Hydroxy-3-nitrobenzaldehyde
- r. 2,3-Dimethylbenzotrile
- s. Pent-1-yn-3-ol
- t. 3-Nitrobenzaldehyde
- u. 3-Ethoxy-4-hydroxybenzaldehyde
- v. 2-Methoxybenzaldehyde
- w. Methyl 4-hydroxybenzoate
- x. Methyl 3-hydroxybenzoate
- y. 3-Aminobenzoic acid
- z. Ethyl 3-aminobenzoate
- aa. Ethyl 4-aminobenzoate
- bb. 3-nitroanisole
- cc. 5-Methyl-2-nitroanisole
- dd. 3-Methylacetanilide

### Reference Books

1. University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N. University of Calcutta, 2003.
2. Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015
3. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education.

**Discipline Specific Elective Course  
(DSE-III and DSE-IV)**

**Any two of the following (Total Credit: 2\*6=12)**

## **1. CHEMISTRY-DSE: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60L**

### **Course objectives and expected outcome:**

- Acquire knowledge about synthesis, application and characterization of glass, cement and ceramic materials.
- Brief knowledge about a few components of batteries, their function, charging and discharging process.
- Gather brief knowledge about silicate industries, dyes and pigments and explosive materials.
- Some basic understanding of catalysis.

### **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.

### **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.

### **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.

### **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.

### **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.

### **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.

### **Chemical explosives:**

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

### **Reference Books:**

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

### **PRACTICALS-DSE LAB: 45L**

- [Practical's knowledge about synthesis and application of fertilizers. Preparation of](#)



pigments, metallic coating and plastic materials.

## **INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE**

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

### **Reference Books:**

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

## **2. CHEMISTRY-DSE: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60L**

### **Course objectives and expected outcome:**

- Students will learn the knowledge about different types of spectroscopic analysis, separation techniques, elemental analysis and bio-molecular detection and conformation.

### **Introduction to spectroscopic methods of analysis:**

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus:

Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

## **Molecular spectroscopy:**

### *Infrared*

#### *spectroscopy:*

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

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

## **Separation techniques**

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

### *Immunoassays and DNA techniques*

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

## **Elemental analysis:**

Mass spectrometry (electrical discharges).

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

Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), Wavelength separation and resolution (dependence on technique), Detection of radiation

(simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

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

**Electroanalytical Methods:** Potentiometry & Voltammetry

**Radiochemical Methods**

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

**Reference books:**

- Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
- Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
- P.W. Atkins: Physical Chemistry.
- G.W. Castellan: Physical Chemistry.
- C.N. Banwell: Fundamentals of Molecular Spectroscopy.
- Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
- W.J. Moore: Physical Chemistry.

**PRACTICALS-DSE      LAB: 45L**

**Course objectives and expected outcome:**

- Students will get hands on training on the different types of spectroscopic analysis, separation techniques, elemental analysis and bio-molecular detection and conformation.

**INSTRUMENTAL              METHODS OF CHEMICAL ANALYSIS**

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)
8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride)
10. Separation of Carbohydrates by HPLC

11. Determination of Caffeine in Beverages by HPLC
12. Potentiometric Titration of a Chloride-Iodide Mixture
13. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple
14. Nuclear Magnetic Resonance
15. Use of fluorescence to do “presumptive tests\_ to identify blood or other body fluids.
16. Use of “presumptive tests\_ for anthrax or cocaine
17. Collection, preservation, and control of blood evidence being used for DNA testing
18. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Ychromosome only or multiple chromosome)
19. Use of sequencing for the analysis of mitochondrial DNA
20. Laboratory analysis to confirm anthrax or cocaine
21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

*At least 10 experiments to be performed.*

**Reference Books:**

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

### **3. CHEMISTRY-DSE: GREEN CHEMISTRY**

**(Credits: Theory-04, Practicals-02)**

**Theory: 60L**

**Course objectives and expected outcome:**

- This course will help to gather the knowledge about green chemistry on the different types of organic materials synthesis and use in social and environment applications.

**Introduction to Green Chemistry**

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry.

Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

**Principles of Green Chemistry and Designing a Chemical synthesis**

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals — different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy

requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization — careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

### **Examples of Green Synthesis/ Reactions**

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzoic acid), Oxidation (of toluene, alcohols).  
Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2- dihydrotriazine derivatives; benzimidazoles.
3. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizzaro reaction, Strecker synthesis, Reformatsky reaction.
4. Selective methylation of active methylene group using dimethylcarbonate: Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of “Clayane”, a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

### **Future Trends in Green Chemistry**

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

### **Reference Books:**

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

Society, Washington (2002).

## **CHEMISTRY PRACTICAL - DSE LAB: 45L**

### **GREEN CHEMISTRY**

#### **Course objectives and expected outcome:**

- This course will help to gather the knowledge about safety materials, renewable energy sources, avoid of waste and photo sensitive materials.

#### **1. Safer starting materials**

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

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

#### **2. Using renewable resources**

Preparation of biodiesel from vegetable oil.

#### **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



#### **4. Use of enzymes as catalysts**

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

#### **Alternative Green solvents**

#### **5. Diels Alder reaction in water**

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

6. Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis (C<sup>2</sup>S<sup>3</sup>) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

#### **Alternative sources of energy**

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

## 10. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

### Reference Books:

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

## 4. CHEMISTRY-DSE: RESEARCH METHODOLOGY FOR CHEMISTRY (Credits: Theory-05, Tutorials-01)

### Theory: 60L

#### Course objectives and expected outcome:

- Students will learn the knowledge about journal searching in internet, H-index of researcher. How to write a publication/book chapter and detailed about the safety materials.

### Literature Survey:

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

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

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

### **Methods of Scientific Research and Writing Scientific Papers:**

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

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

### **Chemical Safety and Ethical Handling of Chemicals:**

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

### **Data Analysis**

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

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

### **Electronics**

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

### **Reference Books**

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2<sup>nd</sup> Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*.



Oxford University Press.

- Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

## **5. CHEMISTRY-DSE: NOVEL INORGANIC SOLIDS (Credits: Theory- 04, Practicals-02)**

### **Theory: 60L**

#### **Course objectives and expected outcome:**

**Students will learn the knowledge about synthesis and modification of inorganic solids, materials of nanostructure, composite and polymer nanocomposite materials for technology applications.**

#### **Synthesis and modification of inorganic solids:**

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

#### **Inorganic solids of technological importance:**

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

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

#### **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 artificial nanomaterials, bionano composites.

#### **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.

#### **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.

### **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.

### **Reference Books:**

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

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## **CHEMISTRY PRACTICAL - DSE LAB: 45L**

### **Course objectives and expected outcome:**

Students will get practical knowledge about synthesis and modification of nanostructure materials.

### **NOVEL INORGANIC SOLIDS**

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

### **Reference Book:**

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

## Generic Elective Syllabus

# Semester I and IV

GE-1/4 [Interdisciplinary for other department]

**GE-1/4 T : ATOMIC STRUCTURE, CHEMICAL PERIODICITY, ACIDS AND BASES, REDOX REACTIONS, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS.**

(Credits: 04 )

Theory: 60L

Section A: Inorganic Chemistry

**Course objectives and expected outcome:** On successful completion of the course students will be able to apply the fundamental principles of measurement, matter, atomic theory, chemical periodicity, general chemical reactivity and solution chemistry to subsequent courses in science.

### Atomic Structure

Bohr's theory for hydrogen atom (simple mathematical treatment), atomic spectra of hydrogen and Bohr's model, Sommerfeld's model, quantum numbers and their significance, Pauli's exclusion principle, Hund's rule, electronic configuration of many-electron atoms, *Aufbau* principle and its limitations.

### Chemical Periodicity

Classification of elements on the basis of electronic configuration: general characteristics of s-, p-, d- and f-block elements. Positions of hydrogen and noble gases. Atomic and ionic radii, ionization potential, electron affinity, and electronegativity; periodic and group-wise variation of above properties in respect of s- and p- block elements.

### Acids and bases

Brønsted–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.

### Redox reactions

Balancing of equations by oxidation number and ion-electron method oxidimetry and reductimetry.

### Section B: Organic Chemistry

**Course objectives and expected outcome:** On successful completion of the course students will be able to apply the fundamental principles of organic chemistry in different parts of learning, They will also know about the stereochemistry of organic molecules.

### Fundamentals of Organic Chemistry

*Electronic displacements:* inductive effect, resonance and hyperconjugation; cleavage of bonds: homolytic and heterolytic; structure of organic molecules on the basis of VBT; nucleophiles electrophiles; reactive intermediates: carbocations, carbanions and free radicals.

## **Stereochemistry**

Different types of isomerism; geometrical and optical isomerism; concept of chirality and optical activity (up to two carbon atoms); asymmetric carbon atom; elements of symmetry (plane and centre); interconversion of Fischer and Newman representations; enantiomerism and diastereomerism, *meso* compounds; *threo* and *erythro*, D and L, *cis* and *trans* nomenclature; CIP Rules: *R/S* (upto 2 chiral carbon atoms) and *E/Z* nomenclature.

## **Nucleophilic Substitution and Elimination Reactions**

*Nucleophilic substitutions*: SN1 and SN2 reactions; eliminations: E1 and E2 reactions (elementary mechanistic aspects); Saytzeff and Hofmann eliminations; elimination vs substitution.

## **Aliphatic Hydrocarbons**

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

*Alkanes*: (up to 5 Carbons). *Preparation*: catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions*: mechanism for free radical substitution: halogenation.

*Alkenes*: (up to 5 Carbons). *Preparation*: elimination reactions: dehydration of alcohols and dehydrohalogenation of alkyl halides; *cis* alkenes (partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions*: *cis*-addition (alkaline KMnO<sub>4</sub>) and *trans*-addition (bromine) with mechanism, addition of HX [Markownikoff's (with mechanism) and anti-Markownikoff's addition], hydration, ozonolysis, oxymercuration-demercuration and hydroboration-oxidation reaction.

*Alkynes*: (up to 5 Carbons). *Preparation*: acetylene from CaC<sub>2</sub> 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<sub>4</sub>, ozonolysis and oxidation with hot alkaline KMnO<sub>4</sub>.

## **Reference Books:**

1. Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
2. Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
3. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.

4. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.
5. Sethi, A. *Conceptual Organic Chemistry*; New Age International Publisher.
6. Parmar, V. S. *A Text Book of Organic Chemistry*, S. Chand & Sons.
7. Madan, R. L. *Organic Chemistry*, S. Chand & Sons.
8. Wade, L. G., Singh, M. S., *Organic Chemistry*.
9. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
10. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
11. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
12. Sen Gupta, Subrata. *Basic Stereochemistry of Organic molecules*.
13. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, Eighth edition, New Age International, 2014.
14. Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

**GE-1/4P LAB: ATOMIC STRUCTURE, CHEMICAL PERIODICITY, ACIDS AND BASES, REDOX REACTIONS, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS**

**(Credits: 02) 45L**

**Course objectives and expected outcome:** Facilitate the learner to make solutions of various molar concentrations. This may include: The concept of the mole; Converting moles to grams; Converting grams to moles; Defining concentration; Dilution of Solutions; Making different molar concentrations. They will also experiences in different type of titration like acid-base, oxidation-reduction titration. They will know about the Qualitative Analysis of Single Solid Organic Compound(s).

**Section A: Inorganic Chemistry –LAB**

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with  $\text{KMnO}_4$ .
3. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$ .
4. Estimation of Fe (II) ions by titrating it with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator.
5. Estimation of Cu (II) ions iodometrically using  $\text{Na}_2\text{S}_2\text{O}_3$ .
6. To find the total hardness of water by EDTA titration.

**Section B: Organic Chemistry- LAB**

*Qualitative Analysis of Single Solid Organic Compound(s)*

Experiment A: Detection of special elements (N, Cl, and S) in organic compounds.

Experiment B: Solubility and Classification (solvents:  $\text{H}_2\text{O}$ , dil. HCl, dil. NaOH)

Experiment C: Detection of functional groups: Aromatic- $\text{NO}_2$ , Aromatic  $-\text{NH}_2$ ,  $-\text{COOH}$ , carbonyl (no distinction of  $-\text{CHO}$  and  $>\text{C}=\text{O}$  needed),  $-\text{OH}$  (phenolic) in solid organic compounds.

Experiments A - C with unknown (at least 6) solid samples containing not more than two of the above type of functional groups should be done.

## **Reference Books:**

1. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta, 2003.
2. Das, S. C., Chakraborty, S. B., *Practical Chemistry*.
3. Mukherjee, K. S. *Text book on Practical Chemistry*, New Oriental Book Agency.
4. Ghosal, Mahapatra & Nad, *An Advanced course in practical Chemistry*, New Central Book Agency.
5. Vogel, A. I. *Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis*, CBS Publishers and Distributors.
6. 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.
7. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

## **Generic Elective Syllabus** **Semester II and III**

### **GE-2/3 [Interdisciplinary for other department]**

**GE2/3T : STATES OF MATTER & CHEMICAL KINETICS, CHEMICAL BONDING & MOLECULAR STRUCTURE, p-BLOCK ELEMENTS**  
**(Credits: Theory-04, Practicals-02)**

**Theory: 60L**

#### ***Section A: Physical Chemistry-I***

**Course objectives and expected outcome:** Facilitate the learner to make knowledge about Kinetic Theory of Gases and Real gases, Liquids, Chemical Kinetics, Conductance.

#### **Kinetic Theory of Gases and Real gases**

Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Rate of effusion

Nature of distribution of velocities, Maxwell's distribution of speed and kinetic energy; Average velocity, root mean square velocity and most probable velocity; Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour; Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states

Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only)

#### **Liquids**

Definition of Surface tension, its dimension and principle of its determination using stalagmometer; Viscosity of a liquid and principle of determination of coefficient of viscosity using Ostwald viscometer; Effect of temperature on surface tension and coefficient of viscosity

of a liquid (qualitative treatment only)

## Chemical Kinetics

Introduction of rate law, Order and molecularity; Extent of reaction; rate constants; Rates of First, second and nth order reactions and their Differential and integrated forms (with derivation); Pseudo first order reactions; Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions Temperature dependence of rate constant; Arrhenius equation, energy of activation; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

## Conductance

Conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Ostwald's dilution law; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations (acid-base) Transport Number and principles of Hittorf's and Moving-boundary method

## Reference Books:

1. Barrow, G.M. *Physical Chemistry* Tata McGraw – Hill (2007).
2. Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
3. Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
4. Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
5. Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
6. Chugh, K.L., Agnish, S.L. *A Text Book of Physical Chemistry* Kalyani Publishers
7. Bahl, B.S., Bahl, A., Tuli, G.D., *Essentials of Physical Chemistry* S. Chand & Co.ltd.
8. Palit, S. R., *Elementary Physical Chemistry* Book Syndicate Pvt. Ltd.
9. Mandal, A. K. *Degree Physical and General Chemistry* Sarat Book House
10. Pahari, S., *Physical Chemistry* New Central Book Agency
11. Pahari, S., Pahari, D., *Problems in Physical Chemistry* New Central Book Agency

## Section B: Inorganic Chemistry-II

**Course objectives and expected outcome:** Upon successful completion students should be able to: know the bonding fundamentals for both ionic and covalent compounds, including electronegativities, bond distances and bond energies using MO diagrams and thermodynamic data and to predict geometries of simple molecules and gain idea of different periodic properties by Comparative study of p-block elements.

## Chemical Bonding and Molecular Structure

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

**Covalent bonding:** VB Approach: Shapes of some inorganic molecules and ions on the basis of

VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of resonance and resonating structures in various inorganic and organic compounds. MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for *s-s*, *s-p* and *p-p* combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods. (including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and NO<sup>+</sup>. Comparison of VB and MO approaches.

### Comparative study of p-block elements:

Group trends in electronic configuration, modification of pure elements, common oxidation states, inert pair effect, and their important compounds in respect of the following groups of elements:

- i) B-Al-Ga-In-Tl      ii) C-Si-Ge-Sn-Pb
- iii) N-P-As-Sb-Bi    iv) O-S-Se-Te      v) F-Cl-Br-I

### Reference Books:

1. Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley.
2. Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
3. Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd.
4. Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008.

## GE2/3P-LAB: STATES OF MATTER & CHEMICAL KINETICS, CHEMICAL BONDING & MOLECULAR STRUCTURE, p-BLOCK ELEMENTS 45L

### Section A: Physical Chemistry-LAB

Course objectives and expected outcome: On successful completion of the course students will be able to:

1. Developed expertise relevant to the professional practice of chemistry.
2. Developed an understanding of the breadth and concepts of physical chemistry.
3. An appreciation of the role of physical chemistry in the chemical sciences.
4. Developed an understanding of the role of the chemist in tasks employing physical chemistry.
5. An understanding of methods employed for problem solving in physical chemistry.
6. Experience in some scientific methods employed in basic and applied physical chemistry.
7. Developed skills in procedures and instrumental methods applied in analytical and practical tasks of physical chemistry.

(Minimum **five** experiments to complete)

(I) Surface tension measurement (use of organic solvents excluded)

- a) Determination of the surface tension of a liquid or a dilute solution using a Stalagmometer
- b) Study of the variation of surface tension of a detergent solution with concentration

(II) Viscosity measurement (use of organic solvents excluded)

- a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer
- b) Study of the variation of viscosity of an aqueous solution with concentration of solute

(III) Study the kinetics of the following reactions

- a) Initial rate method: Iodide-persulphate reaction
- b) Integrated rate method:



- (i) Acid hydrolysis of methyl acetate with hydrochloric acid
- (ii) Compare the strengths of HCl and H<sub>2</sub>SO<sub>4</sub> by studying kinetics of hydrolysis of methyl acetate

(IV) Conductance

Perform the following conductometric titrations: (Any one)

- (i) Strong acid vs. strong base
- (ii) Weak acid vs. strong base

**Reference Books:**

1. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta, 2003.
2. Palit, S.R., *Practical Physical Chemistry* Science Book Agency
3. Mukherjee, N.G., *Selected Experiments in Physical Chemistry* J. N. Ghose & Sons
4. Dutta, S.K., *Physical Chemistry Experiments* Bharati Book Stall

**Section B: Inorganic Chemistry-LAB**

**Course objectives and expected outcome:** Facilitate the learner to experience in qualitative semi micro analysis of mixtures containing four radicals and to understand the chemistry of different reactions and to assign the most probable composition.

**Qualitative semimicro analysis of mixtures containing three radicals. Emphasis should be given to the understanding of the chemistry of different reactions.**

Acid Radicals: Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, NO<sub>2</sub><sup>-</sup>, NO<sub>3</sub><sup>-</sup>, S<sub>2</sub><sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, PO<sub>4</sub><sup>3-</sup>, BO<sub>3</sub><sup>3-</sup>, H<sub>3</sub>BO<sub>3</sub>.

Basic Radicals: Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup>, Sr<sup>2+</sup>, Ba<sup>2+</sup>, Cr<sup>3+</sup>, Mn<sup>2+</sup>, Fe<sup>3+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup>, NH<sub>4</sub><sup>+</sup>.

**Reference Books:**

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