

Draft Syllabus

(Chemistry)

WEF 2019-2020

Raja NL 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

Semester-I

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

CC1T:Physical Chemistry-I

Kinetic Theory and Gaseous state

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 \times , 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, Dietrici); 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)

Chemical Thermodynamics

Zeroth and 1st 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's and 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

c) Chemical kinetics

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and nth 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 ó 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

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 H₂O₂
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

Extra nuclear Structure of atom

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 ψ and ψ^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 upto 30.

Chemical periodicity

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.

Acid-Base reactions

Acid-Base concept: Arrhenius concept, theory of solvent system (in H₂O, NH₃, SO₂ 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.

Redox Reactions and precipitation reactions

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*, 5th 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*, 5th Ed., Oxford University Press (2010).
5. Cotton, F.A., Wilkinson, G. and Gaus, P.L., *Basic Inorganic Chemistry 3rd Ed.*; Wiley India.
6. Sharpe, A.G., *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005.
7. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. *Inorganic Chemistry, Principles of Structure and Reactivity 4th 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 CHEMISTRY (LAB)

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: Na^+ , K^+ , Ca^{2+} , Sr^{2+} , Ba^{2+} , Al^{3+} , Cr^{3+} , $\text{Mn}^{2+}/\text{Mn}^{4+}$, Fe^{3+} , $\text{Co}^{2+}/\text{Co}^{3+}$, Ni^{2+} , Cu^{2+} , Zn^{2+} , Pb^{2+} , Cd^{2+} , Bi^{3+} , $\text{Sn}^{2+}/\text{Sn}^{4+}$, $\text{As}^{3+}/\text{As}^{5+}$, $\text{Sb}^{3+}/\text{Sb}^{5+}$, NH_4^+ , Mg^{2+} .

Anion Radicals: F^- , Cl^- , Br^- , BrO_3^- , I^- , IO_3^- , SCN^- , S^{2-} , SO_4^{2-} , NO_3^- , NO_2^- , PO_4^{3-} , AsO_4^{3-} , BO_3^{3-} , CrO_4^{2-} , $\text{Cr}_2\text{O}_7^{2-}$, $\text{Fe}(\text{CN})_6^{4-}$, $\text{Fe}(\text{CN})_6^{3-}$.

Insoluble Materials: $\text{Al}_2\text{O}_3(\text{ig})$, $\text{Fe}_2\text{O}_3(\text{ig})$, $\text{Cr}_2\text{O}_3(\text{ig})$, SnO_2 , SrSO_4 , BaSO_4 , CaF_2 , 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

Chemical Bonding-I

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 (σ and π bond approach).

Chemical Bonding-II

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.

Radioactivity

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*, 5th Ed., Wiley India Pvt. Ltd., 2008.
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. 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* 3rd 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, 5th 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 CHEMISTRY (LAB)

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 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 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

Basics of Organic Chemistry

Bonding and Physical Properties

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 (sp^3 , sp^2 , 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 σ , σ^* , π , π^* , n ó 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 π 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 α and β ; measurement of delocalization energies in terms of β 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.

General Treatment of Reaction Mechanism I

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).

Stereochemistry I

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_{av} , C_{nh} , C_{nv} , C_n , D_{ch} , 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

1. Separation, based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO₃, 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)

CC-5: Physical Chemistry-II

CC5T: Physical Chemistry-II

Transport processes

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-Hückel 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

Electromotive Force: 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)

Applications of Thermodynamics – I

Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibbs free energy and other thermodynamic state functions; variation of Chemical potential () 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 ó Chemical potential of pure solid and pure liquids, Ideal solution ó 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

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

General Principles of Metallurgy

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

Chemistry of s and p Block Elements

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 XeF_2 , XeF_4 and XeF_6 ; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2 and 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.

Coordination Chemistry-I

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

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 Stereochemistry II

Chirality arising out of stereoaxis: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidenecycloalkanes 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*)ⁿ-*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*).

General Treatment of Reaction Mechanism II

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.

Chemistry of alkenes and alkynes

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)

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

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

Review of concepts studied in the core course:

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

Isolation and characterization of polysachharides.

Proteins: Classification, biological importance; Primary and secondary and tertiary structures of proteins: α -helix and β -pleated sheets, Isolation, characterization, denaturation of proteins.

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

Lipids: Classification. Biological importance of triglycerides and phosphoglycerides and cholesterol; Lipid membrane, Liposomes and their biological functions and underlying

applications. Lipoproteins. Properties, functions and biochemical functions of steroid hormones.

Biochemistry of peptide hormones.

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

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

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

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

Urine: Collection and preservation of samples. 6. Formation of urine. Composition and estimation of constituents of normal and pathological urine.

SEC-P: Analytical Clinical Biochemistry

Credits: 01

Practicals:

Identification and estimation of the following:

1. Carbohydrates ó qualitative and quantitative.
2. Lipids ó 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 ó 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

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-P: Pharmaceutical Chemistry

Credits: 01

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

Credits 02

SEC-T: BASIC ANALYTICAL CHEMISTRY

Credits 01

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

Credits 01

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 (Fe^{3+} and 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

CC8T: Physical Chemistry-III

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, CO₂, 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

Electrical Properties of molecules

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

Quantum Chemistry

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:

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

Coordination Chemistry-II

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 $3d^1$ to $3d^9$ ions. Racah parameter. Selection rules for electronic spectral transitions; spectrochemical series of ligands; charge transfer spectra (elementary idea).

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 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

Iodo-/ Iodimetric Titrations

1. Estimation of Cu(II)
2. Estimation of Vitamin C
3. Estimation of (i) arsenite and (ii) antimony in tartar-emetic 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

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); *ipso* substitution.

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

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 α -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 α,β -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).

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., Guiliano, 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.

CC10P: Organic Chemistry-III –Lab

Credits 02

Experiment -1: Qualitative Analysis of Single Solid Organic Compounds

- a) Detection of special elements (N, S, Cl, Br) by Lassaigne's test
- b) Solubility and classification (solvents: H₂O, 5% HCl, 5% NaOH and 5% NaHCO₃)
- c) Detection of the following functional groups by systematic chemical tests: aromatic amino (-NH₂), aromatic nitro (-NO₂), amido (-CONH₂, including imide), phenolic -OH, carboxylic acid (-COOH), carbonyl (-CHO and >C=O); only one test for each functional group is to be reported.
- d) Melting point of the given compound
- e) Preparation, purification and melting point determination of a crystalline derivative of the given compound
- f) 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:

1. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, 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. Clarke, H. T., *A Handbook of Organic Analysis (Qualitative and Quantitative)*, Fourth Edition, CBS Publishers and Distributors (2007).
6. *Practical Workbook Chemistry (Honours)*, UGBS, Chemistry, University of Calcutta, 2015.

Skill Enhancement Course (SEC)

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

1. SEC: CHEMISTRY OF COSMETICS & PERFUMES Credit 02

SEC-T: CHEMISTRY OF COSMETICS & PERFUMES Credit 01

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 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 Credit 01

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. Cremlyn: *Pesticides*, John Wiley.

3. SEC: FUEL CHEMISTRY

Credits 02

SEC-T: FUEL CHEMISTRY

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, pore 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:

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.

Semester-V

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

Physical Chemistry-IV

CC11T: Physical Chemistry-IV

Molecular Spectroscopy

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

Photochemistry

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, H₂-Br₂ reaction, dimerisation of anthracene; photosensitised reactions, quenching; Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence

Surface phenomenon

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; Heterogeneous 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 Schulz-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:

List of Practical

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 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

Credits 04

Nitrogen compounds

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.

Rearrangements

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 benzdine rearrangement.

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

The Logic of Organic Synthesis

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.

Organic Spectroscopy

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 λ_{\max} for the following systems: conjugated diene, α,β -unsaturated aldehydes and ketones (alicyclic, homoannular and heteroannular); extended conjugated systems (dienes, aldehydes and ketones); relative positions of λ_{\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

Credits 02

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:

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:

É Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.

É Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.

É Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).

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

PRACTICAL-DSE LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY

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:

- É McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
- É Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- É Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- É Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007).
- É Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- É Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- É Noggle, J. H. *Physical Chemistry on a Microcomputer*. Little Brown & Co. (1985).
- É 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:

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:

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

PRACTICALS- DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

(i) Paper chromatographic separation of Fe³⁺, Al³⁺, and Cr³⁺.

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

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

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

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

II. Solvent

Extractions:

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

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

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

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

5. Analysis of soil:

(i) Determination of pH of

soil. (ii) Total soluble salt

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

6. Ion exchange:

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

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

III Spectrophotometry

1. Determination of pK_a values of indicator using spectrophotometry.

2 Structural characterization of compounds by infrared spectroscopy.

3 Determination of dissolved oxygen in water.

4 Determination of chemical oxygen demand (COD).

5 Determination of Biological oxygen demand (BOD).

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

Reference Books:

É Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .

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

É Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.

É Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.

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

É Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.

É Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.

- Ditts, R.V. Analytical Chemistry – Methods of separation.

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

Theory:

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

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

Reference Books:

- A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.

- J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
- Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

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

Theory:

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

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: POLYMER CHEMISTRY

1. Polymer synthesis

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

Polymer characterization

1. Determination of molecular weight by viscometry: (a) Polyacrylamide-aq. NaNO_2 solution (b) (Poly vinyl propylidene (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

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

*at least 7 experiments to be carried out.

Reference Books:

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

5. CHEMISTRY-DSE: INDUSTRIAL CHEMICALS AND ENVIRONMENT (Credits: Theory-04, Practicals-02)

Theory:

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 SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures.

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

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

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

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

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:

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

CHEMISTRY PRACTICAL - DSE LAB: 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 (AgNO_3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-} , HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2 .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Reference Books:

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

Semester-VI

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

CC13T: INORGANIC CHEMISTRY-V

Bioinorganic Chemistry

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^+ ,

K^+ , Mg^{2+} , Ca^{2+} , $Fe^{3+}/^{2+}$, $Cu^{2+}/^+$, and Zn^{2+}). Metal ion transport across biological membrane Na^+/K^+ ion pump. Dioxygen molecule in life. Dioxygen management proteins: Haemoglobin, Myoglobin, Hemocyanine and Hemerythrin. Electron transfer proteins: Cytochromes and Ferredoxins. Hydrolytic 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)

Organometallic Chemistry

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. π -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.

Catalysis by Organometallic Compounds

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.

Reaction Kinetics and Mechanism

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

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)₃ (aluminium oxinate)
4. Estimation of chloride

Spectrophotometry

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

Reference Books

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

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

CC14T - Organic Chemistry V

Organic Chemistry V (Theory)

4 Credit

Carbocycles and Heterocycles

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.

Cyclic Stereochemistry

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 (E2, E1), nucleophilic substitution (SN1, SN2, SNi, NGP), merged substitution-elimination; rearrangements; oxidation of cyclohexanol, esterification, saponification, lactonisation, epoxidation, pyrolytic syn elimination and fragmentation reactions.

Pericyclic reactions

Mechanism, stereochemistry, regioselectivity in case of

1. Electrocyclic reactions: FMO approach involving 4 - and 6 -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.

Carbohydrates

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, HNO₃ oxidation, selective oxidation of terminal δ CH₂OH of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; steppingóup (Kiliani-Fischer method) and steppingódown (Ruffó & Wohló 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, acetamidomalonic 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); complementary base pairing in DNA.

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; Synthesis and applications of: Azo dyes ó Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes -Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes ó Phenolphthalein and Fluorescein; Natural dyes ó 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)

2 Credit

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 δ -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-Dimethylbenzonitrile
- 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:

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:

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

PRACTICALS-DSE LAB: 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:

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

2. CHEMISTRY-DSE: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

(Credits: Theory-04, Practicals-02)

Theory:

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 ó 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:

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

PRACTICALS-DSE LAB: 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 (Y-chromosome only or multiple chromosome)
19. Use of sequencing for the analysis of mitochondrial DNA
20. Laboratory analysis to confirm anthrax or cocaine
21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

At least 10 experiments to be performed.

Reference Books:

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

3. CHEMISTRY-DSE: GREEN CHEMISTRY

(Credits: Theory-04, Practicals-02)

Theory:

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 ó 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 ó 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 O_2 as 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:

1. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry,

2. Anamalaya Publishers (2005).

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

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

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

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

CHEMISTRY PRACTICAL - DSE LAB: GREEN CHEMISTRY

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

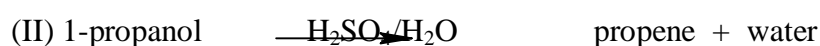
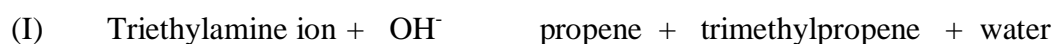
Preparation of biodiesel from vegetable oil.

Avoiding waste

Principle of atom economy.

Use of molecular model kit to simulate 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 CO₂ prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis (C²S³) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

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

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

Reference Books:

- É Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
- É Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
- É Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- É 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).
- É Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- É Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
- É Pavia, D. L. Lamponan, G. H. &Kriz, G.S. *W B Introduction to organic laboratory*

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

Theory:

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*. 2nd Ed. Prentice-Hall, Harlow.
 - Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
 - Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
 - Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
 - Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
 - Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
 - OSU safety manual 1.01.

5. CHEMISTRY-DSE: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Theory:

Synthesis and modification of inorganic solids:

Conventional heat and beat 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 fullerides, 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 antisical 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, 5th 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

CHEMISTRY PRACTICAL - DSE LAB: 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 III

GE-1/3 [Interdisciplinary for other department]

GE-1/3 T : ATOMIC STRUCTURE, CHEMICAL PERIODICITY, ACIDS AND BASES, REDOX REACTIONS, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS.

(Credits: 04)

Theory:

Section A: Inorganic Chemistry

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

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 KMnO₄) 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 CaC₂ 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 KMnO₄, ozonolysis and oxidation with hot alkaline KMnO₄.

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 I)*, 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-1/3P LAB: ATOMIC STRUCTURE, CHEMICAL PERIODICITY, ACIDS AND BASES, REDOX REACTIONS, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS
(Credits: 02)

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 KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.
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: H_2O , dil. HCl, dil. NaOH)

Experiment C: Detection of functional groups: Aromatic- NO_2 , Aromatic - NH_2 , -COOH, carbonyl (no distinction of CHO and $>\text{C}=\text{O}$ needed), -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 IV**

GE-2/4 [Interdisciplinary for other department]

**GE2/4T : STATES OF MATTER & CHEMICAL KINETICS, CHEMICAL BONDING & MOLECULAR STRUCTURE, p-BLOCK ELEMENTS
(Credits: Theory-04, Practicals-02)**

Theory:

Section A: Physical Chemistry-I

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; Andrews 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

Chemical Bonding and Molecular Structure

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

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

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

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.

GE2/4P-LAB: STATES OF MATTER & CHEMICAL KINETICS, CHEMICAL BONDING & MOLECULAR STRUCTURE, p-BLOCK ELEMENTS

Section A: Physical Chemistry-LAB

(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 H₂SO₄ 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

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

Acid Radicals: Cl⁻, Br⁻, I⁻, NO₂⁻, NO₃⁻, S₂⁻, SO₄²⁻, PO₄³⁻, BO₃³⁻, H₃BO₃.

Basic Radicals: Na⁺, K⁺, Ca²⁺, Sr²⁺, Ba²⁺, Cr³⁺, Mn²⁺, Fe³⁺, Ni²⁺, Cu²⁺, NH₄⁺.

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).