

Chemistry (Hons) CBCS Syllabus

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1. Scheme for CBCS Curriculum

1.1 Credit Distribution across Courses

Credits

Course Type	Total Papers	Theory + Practical	Theory*
Core Course	14	14*4 =56	14*5 =70
		14*2 =28	14*1=14
Discipline Specific Electives	4	4*4=16	4*5=20
		4*2=8	4*1=4
Generic Electives	4	4*4=16	4*5=20
		4*2=8	4*1=4
Ability Enhancement Language Courses	2	2*2=4	2*2=4
Skill Enhancement Courses	2	2*2=4	2*2=4
Total	22	140	140

*Tutorials of 1 Credit will be conducted in case there is no practical component

1.2 Scheme for CBCS Curriculum

Semester	Course Name	Course Detail	Credits
I	Ability Enhancement Compulsory Course - I	English communication / Environmental Science	2
	Core course - I	Organic Chemistry I	4
	Core course - I Practical	Organic Chemistry I	2
	Core course - II	Physical Chemistry I	4
	Core course - II Practical	Physical Chemistry I	2
	Genetic Elective - 1	TBD	4
	Generic Elective - 1 Practical	TBD	2
II	Ability Enhancement Compulsory Course - II	English communication / Environmental Science	2
	Core course - III	Inorganic Chemistry I	4
	Core course - III Practical	Inorganic Chemistry I	2
	Core course - IV	Organic Chemistry II	4
	Core course - IV Practical	Organic Chemistry II	2
	Generic Elective - 2	TBD	4
	Generic Elective - 2 Practical	TBD	2

III	Core course - V	Physical Chemistry II	4
	Core course - V Practical	Physical Chemistry II	2
	Core course - VI	Inorganic Chemistry II	4
	Core course - VI Practical	Inorganic Chemistry II	2
	Core course - VII	Organic Chemistry III	4
	Core course - VII Practical	Organic Chemistry III	2
	Skill Enhancement Course - 1	TBD	2
	Generic Elective - 3	TBD	4
	Generic Elective - 3 Practical	TBD	2
III	Core course - V	Physical Chemistry II	4
	Core course - V Practical	Physical Chemistry II	2
	Core course - VI	Inorganic Chemistry II	4
	Core course - VI Practical	Inorganic Chemistry II	2
	Core course - VII	Organic Chemistry III	4
	Core course - VII Practical	Organic Chemistry III	2
	Skill Enhancement Course - 1	TBD	2
	Generic Elective - 3	TBD	4
	Generic Elective - 3 Practical	TBD	2
IV	Core course - VIII	Physical Chemistry III	4
	Core course - VIII Practical	Physical Chemistry III	2
	Core course - IX	Inorganic Chemistry III	4
	Core course - IX Practical	Inorganic Chemistry III	2
	Core course - X	Organic Chemistry IV	4
	Core course - X Practical	Organic Chemistry IV	2
	Skill Enhancement Course-2	TBD	2
	Generic Elective - 4	TBD	4
	Generic Elective - 4 Practical	TBD	2
V	Core course - XI	Inorganic Chemistry IV	4
	Core course - XI Practical	Inorganic Chemistry IV	2
	Core course - XII	Organic Chemistry V	4
	Core course - XII Practical	Organic Chemistry V	2
	Discipline Specific Elective - 1	TBD	4
	Discipline Specific Elective - 1 Practical	TBD	2
	Discipline Specific Elective - 2	TBD	4
	Discipline Specific Elective - 2 Practical	TBD	2
VI	Core course - XIII	Inorganic Chemistry V	4
	Core course - XIII Practical	Inorganic Chemistry V	2
	Core course - XIV	Physical Chemistry IV	4
	Core course - XIV Practical	Physical Chemistry IV	2
	Discipline Specific Elective - 3	TBD	4
	Discipline Specific Elective - 3 Practical	TBD	2
	Discipline Specific Elective - 4	TBD	4
	Discipline Specific Elective - 4 Practical	TBD	2

1.3 Discipline Specific Electives

Advanced Physical Chemistry	Green Chemistry	Analytical Methods in Chemistry
Polymer Chemistry		

1.4 Skill Enhancement Courses

Basic Analytical Chemistry; Pharmaceutical Chemistry.

2. Core Subjects Syllabus

2.1 Core T1 - Organic Chemistry I

4 Credits

Bonding and Physical Properties

1. 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)
2. Electronic displacements: inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.
3. MO theory: Qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ , σ^* , π , π^* , n – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of 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.
4. 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

1. 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.
2. 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

1. 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.
2. Concept of chirality and symmetry: symmetry elements and point groups (C_v , C_{nh} , C_{nv} , C_n , D_h , D_{nh} , D_{nd} , D_n , S_n , C_s , C_i); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).
3. 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
4. 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

- ▶ Clayden, J., Greeves, N. & Warren, S. Organic Chemistry, Second edition, Oxford University Press, 2012
- ▶ Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited.
- ▶ Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
- ▶ Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd., (Pearson Education).
- ▶ Fleming, I. Molecular Orbitals and Organic Chemical Reactions, Reference/Student Edition, Wiley, 2009.
- ▶ James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003.
- ▶ Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005.

2.2 Core P1 – Organic Chemistry I Lab.

2 Credits

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.

Determination of boiling point

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]

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

- ▶ Bhattacharyya, R. C, A Manual of Practical Chemistry.
- ▶ Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.
- ▶ Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
- ▶ Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).

2.3 Core T2 - Physical Chemistry I I

4 Credits

Kinetic Theory and Gaseous state

1. 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
2. Maxwell's distribution of speed and energy: Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy $\geq \epsilon$, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases
3. 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

1. 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
2. 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
3. Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of 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.
4. 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

Chemical kinetics

1. 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)
2. Role of T and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)
3. 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
4. Autocatalysis; periodic reactions

Reference Books

- Atkins, P. W. & Paula, J. de Atkins' Physical Chemistry, Oxford University Press

- ▶ Castellan, G. W. Physical Chemistry, Narosa
- ▶ McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
- ▶ Engel, T. & Reid, P. Physical Chemistry, Pearson
- ▶ Levine, I. N. Physical Chemistry, Tata McGraw-Hill
- ▶ Maron, S. & Prutton Physical Chemistry
- ▶ Ball, D. W. Physical Chemistry, Thomson Press
- ▶ Mortimer, R. G. Physical Chemistry, Elsevier
- ▶ Laidler, K. J. Chemical Kinetics, Pearson
- ▶ Glasstone, S. & Lewis, G.N. Elements of Physical Chemistry
- ▶ Rakshit, P.C., Physical Chemistry Sarat Book House
- ▶ Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata-McGraw-Hill
- ▶ Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas
- ▶ Clauze & Rosenberg, Chemical Thermodynamics

2.4 Core P2 - Physical Chemistry I Lab I

2 Credits

List of Practical

1. Determination of pH of unknown solution (buffer), by color matching method
2. Determination of heat of neutralization of a strong acid by a strong base
3. Study of kinetics of acid-catalyzed hydrolysis of methyl acetate
4. Study of kinetics of decomposition of H₂O₂
5. Determination of heat of solution of oxalic acid from solubility measurement

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.

2.5 Core T3 - Inorganic Chemistry II

4 Credits

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 AllredRochow'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). 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.

Reference Books

- ▶ Lee, J. D. Concise Inorganic Chemistry ELBS, 1991.
- ▶ Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970.
- ▶ Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications, 1962. ▶
- ▶ Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
- ▶ Cotton, F.A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry 3rd Ed.; Wiley India.
- ▶ Sharpe, A.G., Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005.

- ▶ Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- ▶ Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
- ▶ Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998).
- ▶ Winter, M. J., The Orbitron, <http://winter.group.shef.ac.uk/orbitron/> (2002). An illustrated gallery of atomic and molecular orbitals.
- ▶ Burgess, J., Ions in solution: basic principles of chemical interactions. Ellis Horwood (1999).

2.6 Core P3 - Inorganic Chemistry I Lab

2 Credits

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.

2.7 Core T4 - Organic Chemistry II

4 Credits

Stereochemistry II

1. 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.
2. 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 R_e/S_i descriptors; pro- r and pro- s descriptors of ligands on propseudoasymmetric centre.
3. 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, 4. 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

1. Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.
2. 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.
3. 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.
4. 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 isotope effect (k_H/k_D); principle of microscopic reversibility; Hammond's postulate.

Substitution and Elimination Reactions

1. Free-radical substitution reaction: halogenation of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.
2. Nucleophilic substitution reactions: substitution at sp^3 centre: mechanisms (with evidence), relative rates & stereochemical features: SN^1 , SN^2 , SN^2' , SN^1' (allylic rearrangement) and SN_i ; 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]
3. Elimination reactions: $E1$, $E2$, $E1CB$ and E_i (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

- ▶ Clayden, J., Greeves, N., Warren, S. Organic Chemistry, Second edition, Oxford University Press 2012.
- ▶ Sykes, P.A guidebook to Mechanism in Organic Chemistry, Pearson Education, 2003.
- ▶ Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited.

- ▶ Carey, F. A. & Giuliano, R. M. Organic Chemistry, Eighth edition, McGraw Hill Education, 2012.
- ▶ Loudon, G. M. Organic Chemistry, Fourth edition, Oxford University Press, 2008.
- ▶ Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
- ▶ Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
- ▶ Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Finar, I. L. Organic Chemistry (Volume 1) Pearson Education.
- ▶ Graham Solomons, T.W., Fryhle, C. B. Organic Chemistry, John Wiley & Sons, Inc.
- ▶ James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003.
- ▶ Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005.
- ▶ Maskill, H., Mechanisms of Organic Reactions, Oxford Chemistry Primer, Oxford University Press.

2.8 Core P4 - Organic Chemistry II Lab.

2 Credits

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

- ▶ Vogel, A. I. Elementary Practical Organic Chemistry, Part 1: Small scale Preparations, CBS Publishers and Distributors.
- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N. University of Calcutta, 2003.

- ▶ Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
- ▶ Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012).
- ▶ Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- ▶ Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015.

2.9 Core T5 - Physical Chemistry II

4 Credits

Transport processes

1. Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties
2. 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
3. Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye –Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations
4. Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule

Applications of Thermodynamics – I

1. Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential (μ) 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
2. 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
3. Nernst's distribution law; Application- (finding out K_{eq} using Nernst dist law for $KI + I_2 = KI_3$ and dimerization of benzene.

4. Chemical potential and other properties of ideal substances- pure and mixtures:
- 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
 - Condensed Phase – Chemical potential of pure solid and pure liquids, Ideal solution – Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution; Choice of standard states of solids and liquids

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 , px and px^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

Reference Books

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

2.10 Core P5 - Physical Chemistry II Lab.

2 Credits

List of Practical

1. Study of viscosity of unknown liquid (glycerol, sugar) with respect to water
2. Determination of partition coefficient for the distribution of I₂ between water and CCl₄
3. Determination of K_{eq} for KI + I₂ = KI₃, using partition coefficient between water and CCl₄
4. Conductometric titration of an acid (strong, weak/ monobasic, dibasic) against base strong
5. Study of saponification reaction conductometrically
6. Verification of Ostwald's dilution law and determination of K_a of weak acid

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.

2.11 Core T6 - Inorganic Chemistry II

4 Credits

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 nonequivalent 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 H₂, Li₂, Be₂, B₂, C₂, N₂, O₂, F₂, and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO, NO⁺, CN⁻, HF, BeH₂, CO₂ and H₂O. 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

1. Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers.

2. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes.

3. Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

Reference Books

- ▶ Lee, J. D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
- ▶ Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- ▶ Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970.
- ▶ Porterfield, H. W., Inorganic Chemistry, Second Edition, Academic Press, 2005.
- ▶ Purecell, K.F. and Kotz, J.C., An Introduction to Inorganic Chemistry, Saunders: Philadelphia, 1980.
- ▶ Cotton, F.A., Wilkinson, G., & Gaus, P.L. Basic Inorganic Chemistry 3rd Ed.; Wiley India.
- ▶ Gillespie, R. J. and Hargittai, I., The VSEPR Model of Molecular Geometry, Prentice Hall (1992).
- ▶ Albright, T., Orbital interactions in chemistry, John Wiley and Sons (2005).
- ▶ Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998).
- ▶ Miessler, G. L., Fischer, P. J., Tarr, D. A., Inorganic Chemistry, Pearson, 5th Edition.

2.12 Core P6 - Inorganic Chemistry II Lab.

2 Credits

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.

Reference Books

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

Chemistry of alkenes and alkynes

1. 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.

2. 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 nonterminal alkynes.

Aromatic Substitution

1. 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.

2. Nucleophilic aromatic substitution: addition-elimination mechanism and evidences in favour of it; SN1 mechanism; cine substitution (benzyne mechanism), structure of benzyne.

Carbonyl and Related Compounds

1. 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, LiAlH₄, NaBH₄, MPV, Oppenauer, Bouveault-Blanc, acyloin condensation; oxidation of alcohols with PDC and PCC; periodic acid and lead tetraacetate oxidation of 1,2-diols.

2. 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, SeO₂ (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.

3. 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.

4. 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.

5. Substitution at sp^2 carbon (C=O system): mechanism (with evidence): BAC2, AAC2, AAC1, AAL1 (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.

Reference Books

- ▶ Clayden, J., Greeves, N., Warren, S. Organic Chemistry, Second edition, Oxford University Press 2012.
- ▶ Sykes, P.A guidebook to Mechanism in Organic Chemistry, Pearson Education, 2003.
- ▶ Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited.
- ▶ Carey, F. A., Giuliano, R. M. Organic Chemistry, Eighth edition, McGraw Hill Education, 2012.
- ▶ Loudon, G. M. Organic Chemistry, Fourth edition, Oxford University Press, 2008.
- ▶ Norman, R.O. C., Coxon, J. M. Principles of Organic Synthesis, Third Edition, Nelson Thornes, 2003.
- ▶ Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Pearson Education.
- ▶ Graham Solomons, T.W., Fryhle, C. B. Organic Chemistry, John Wiley & Sons, Inc.

- ▶ March, J. Advanced Organic Chemistry, Fourth edition, Wiley.
- ▶ Jenkins, P. R., Organometallic Reagents in Synthesis, Oxford Chemistry Primer, Oxford University Press.
- ▶ Ward, R. S., Bifunctional Compounds, Oxford Chemistry Primer, Oxford University Press.

2.14 Core P7 - Organic Chemistry III Lab.

2 Credits

Qualitative Analysis of Single Solid Organic Compounds

1. Detection of special elements (N, S, Cl, Br) by Lassaigne's test
2. Solubility and classification (solvents: H₂O, 5% HCl, 5% NaOH and 5% NaHCO₃)
3. Detection of the following functional groups by systematic chemical tests:
4. 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.
5. Melting point of the given compound
6. Preparation, purification and melting point determination of a crystalline derivative of the given compound
7. 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

Reference Books

- ▶ Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.
- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N. University of Calcutta, 2003.
- ▶ Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009).
- ▶ Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012).
- ▶ Clarke, H. T., A Handbook of Organic Analysis (Qualitative and Quantitative), Fourth Edition, CBS Publishers and Distributors (2007).
- ▶ Practical Workbook Chemistry (Honours), UGBS, Chemistry, University of Calcutta, 2015.

2.15 Core T8 - Physical Chemistry III

4 Credits

Application of Thermodynamics – II

1. 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
2. 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
 3. First order phase transition and Clapeyron equation; Clausius-Clapeyron equation - derivation and use; Liquid vapour equilibrium for two component systems; Phenol-water system
 4. Three component systems, water-chloroform-acetic acid system, triangular plots
 5. 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

1. 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
2. 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 SbO/Sb₂O₃ electrodes
3. 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)
4. 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

1. 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

2. 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)
3. LCAO and HF-SCF: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+ ; Bonding and antibonding orbitals; Qualitative extension to H_2 ; Comparison of LCAO-MO and VB treatments of H_2 and their limitations; Hartree-Fock method development, SCF and configuration interaction (only basics)

Reference Books

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

2.16 Core P8 - Physical Chemistry III Lab.

2 Credits

List of Practical

1. Determination of solubility of sparingly soluble salt in water, in electrolyte with common ions and in neutral electrolyte (using common indicator)
2. Potentiometric titration of Mohr's salt solution against standard $K_2Cr_2O_7$ solution
3. Determination of K_{sp} for AgCl by potentiometric titration of $AgNO_3$ solution against standard KCl solution
4. Effect of ionic strength on the rate of Persulphate – Iodide reaction
5. Study of phenol-water phase diagram
6. pH-metric titration of acid (mono- and di-basic) against strong base

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.

2.17 Core T9 - Inorganic Chemistry III

4 Credits

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, pseudohalogen, 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.

Reference Books

- ▶ Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- ▶ Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
- ▶ Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., Advanced Inorganic Chemistry 6th Ed. 1999., Wiley.
- ▶ Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010.
- ▶ Purecell, K.F. and Kotz, J.C., An Introduction to Inorganic Chemistry, Saunders: Philadelphia, 1980.
- ▶ Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998).

2.18 Core P9 - Inorganic Chemistry III Lab.

r2 Credits

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

Reference Books

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

Nitrogen compounds

1. 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.
2. 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.
3. Alkyl nitrile and isonitrile: preparation and reaction (with mechanism): Thorpe nitrile condensation, von Richter reaction.
4. 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:

1. Rearrangement to electron-deficient carbon: Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt-Eistert synthesis, benzilbenzilic acid rearrangement, Demjanov rearrangement, Tiffeneau-Demjanov rearrangement.
2. Rearrangement to electron-deficient nitrogen: rearrangements: Hofmann, Curtius, Lossen, Schmidt and Beckmann.
3. Rearrangement to electron-deficient oxygen: Baeyer-Villiger oxidation, cumene hydroperoxide-phenol rearrangement and Dakin reaction.
4. Aromatic rearrangements: Migration from oxygen to ring carbon: Fries rearrangement and Claisen rearrangement.
5. Migration from nitrogen to ring carbon: Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement and benzidine rearrangement.
6. Rearrangement reactions by green approach: Fries rearrangement, Claisen rearrangement, Beckmann rearrangement, Baeyer-Villiger oxidation.

The Logic of Organic Synthesis

1. 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).\
2. Strategy of ring synthesis: thermodynamic and kinetic factors; synthesis of large rings, application of high dilution technique.

3. 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

1. 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.

2. IR Spectroscopy: introduction; modes of molecular vibrations (fundamental and nonfundamental); 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.

3. 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.

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

Reference Books

- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Norman, R.O. C., Coxon, J. M. Principles of Organic Synthesis, Third Edition, Nelson Thornes, 2003.

- ▶ Clayden, J., Greeves, N., Warren, S., Organic Chemistry, Second edition, Oxford University Press 2012.
- ▶ Silverstein, R. M., Bassler, G. C., Morrill, T. C. Spectrometric Identification of Organic Compounds, John Wiley and Sons, INC, Fifth edition.
- ▶ Kemp, W. Organic Spectroscopy, Palgrave.
- ▶ Pavia, D. L. et al. Introduction to Spectroscopy, 5th Ed. Cengage Learning India Ed. (2015).
- ▶ Dyer, J. Application of Absorption Spectroscopy of Organic Compounds, PHI Private Limited
- ▶ March, J. Advanced Organic Chemistry, Fourth edition, Wiley.
- ▶ Harwood, L. M., Polar Rearrangements, Oxford Chemistry Primer, Oxford University Press.
- ▶ Bailey, Morgan, Organonitrogen Chemistry, Oxford Chemistry Primer, Oxford University Press.
- ▶ Warren, S. Organic Synthesis the Disconnection Approach, John Wiley and Sons.
- ▶ Warren, S., Designing Organic Synthesis, Wiley India, 2009.
- ▶ Carruthers, W. Modern methods of Organic Synthesis, Cambridge University Press.
- ▶ Willis, C. A., Wills, M., Organic Synthesis, Oxford Chemistry Primer, Oxford University Press.

2.20 Core P10 - Organic Chemistry IV Lab.

2 Credits

List of Practical

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

Reference Books

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

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

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

2.22 Core P11 - Inorganic Chemistry IV Lab.

2 Credits

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 λ_{max} of [Mn(acac)₃] and [Fe(acac)₃] complexes

Reference Books

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

2.23 Core T12 - Organic Chemistry V

V4 Credits

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, FeistBenary 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: Skrap, 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 4π - and 6π -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 -CH₂OH of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping-up (Kiliani-Fischer method) and stepping-down (Ruff's & Wohl's methods) of aldoses; end-group-interchange of aldoses; acetonide (isopropylidene) and benzylidene protections; ring-size determination; Fischer's proof of configuration of (+)-glucose.
2. Disaccharides: Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar.
3. Polysaccharides: starch (structure and its use as an indicator in titrimetric analysis).

Biomolecules

1. Amino acids: synthesis with mechanistic details: Strecker, Gabriel, acetamido malonic ester, azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine; isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids.

2. Peptides: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using N-protection & C-protection, solid-phase (Merrifield) synthesis; peptide sequence: C-terminal and N-terminal unit determination (Edman, Sanger & 'dansyl' methods); partial hydrolysis; specific cleavage of peptides: use of CNBr.

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

Reference Books

- ▶ Clayden, J., Greeves, N., Warren, S. Organic Chemistry, Second edition, Oxford University Press 2012.
- ▶ Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London.
- ▶ Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited.
- ▶ Sen Gupta, Subrata. Basic Stereochemistry of Organic molecules.
- ▶ Kalsi, P. S. Stereochemistry Conformation and Mechanism, Eighth edition, New Age International, 2014.
- ▶ Fleming, I. Molecular Orbitals and Organic Chemical reactions, Reference/Student Edition, Wiley, 2009.
- ▶ Fleming, I. Pericyclic Reactions, Oxford Chemistry Primer, Oxford University Press.
- ▶ Gilchrist, T. L. & Storr, R. C. Organic Reactions and Orbital symmetry, Cambridge University Press.
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Loudon, G. M. Organic Chemistry, Fourth edition, Oxford University Press.
- ▶ James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003.
- ▶ Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005.
- ▶ Davis, B. G., Fairbanks, A. J., Carbohydrate Chemistry, Oxford Chemistry Primer, Oxford University Press.
- ▶ Joule, J. A. Mills, K. Heterocyclic Chemistry, Blackwell Science.
- ▶ Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Wiley & Sons (1976).
- ▶ Gilchrist, T. L. Heterocyclic Chemistry, 3rd edition, Pearson.
- ▶ Bansal, R. K. Heterocyclic Chemistry, New Age International Publishers.
- ▶ Davies, D. T., Heterocyclic Chemistry, Oxford Chemistry Primer, Oxford University Press.

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 labelled peaks in the ^1H 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, $\text{C}\equiv\text{C}$, $\text{C}\equiv\text{N}$ stretching frequencies; characteristic bending vibrations are included).
3. The students must record full spectral analysis of at least 15 (fifteen) compounds from the following list:
 - a. 4-Bromoacetanilide
 - b. 2-Bromo-4'-methylacetophenone
 - c. Vanillin
 - d. 2-Methoxyacetophenone
 - e. 4-Aminobenzoic acid
 - f. Salicylamide
 - g. 2-Hydroxyacetophenone
 - h. 1,3-Dinitrobenzene
 - i. Benzylacetate
 - j. trans-4-Nitrocinnamaldehyde
 - k. Diethyl fumarate
 - l. 4-Nitrobenzaldehyde
 - m. 4-Methylacetanilide
 - n. Mesityl oxide
 - o. 2-Hydroxybenzaldehyde
 - p. 4-Nitroaniline
 - q. 2-Hydroxy-3-nitrobenzaldehyde
 - r. 2,3-Dimethylbenzotrile
 - s. Pent-1-yn-3-ol
 - t. 3-Nitrobenzaldehyde
 - u. 3-Ethoxy-4-hydroxybenzaldehyde
 - v. 2-Methoxybenzaldehyde
 - w. Methyl 4-hydroxybenzoate
 - x. Methyl 3-hydroxybenzoate
 - y. 3-Aminobenzoic acid

- z. Ethyl 3-aminobenzoate
- aa. Ethyl 4-aminobenzoate
- bb. 3-nitroanisole
- cc. 5-Methyl-2-nitroanisole
- dd. 3-Methylacetanilide

Reference Books

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

2.25 Core T13 - Inorganic Chemistry V

4 Credits

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+} , $\text{Fe}^{3+/2+}$, $\text{Cu}^{2+/+}$, 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

- ▶ Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
- ▶ Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006.
- ▶ Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.
- ▶ Cotton, F.A., Wilkinson, G., Murrillo, C. A., Bochmann, M., Advanced Inorganic Chemistry 6th Ed. 1999., Wiley.
- ▶ Bertini, I., Gray, H. B., Lippard, S.J., Valentine, J. S., Viva, 2007.
- ▶ Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
- ▶ Purecell, K.F. and Kotz, J.C., An Introduction to Inorganic Chemistry, Saunders: Philadelphia, 1980.
- ▶ Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- ▶ Collman, J. P. et al. Principles and Applications of Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
- ▶ Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. New York, NY: John Wiley, 2000.

2.26 Core P13 – Inorganic Chemistry V Lab.

V 2 Credits

Qualitative semimicro analysis

Qualitative semimicro analysis of mixtures containing four radicals. Emphasis should 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^{2+} , $\text{Sn}^{2+}/\text{Sn}^{4+}$, $\text{As}^{3+}/\text{As}^{5+}$, $\text{Sb}^{3+}/\text{Sb}^{5+}$, NH_4^+ , Mg^+ . 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.

2.27 Core T14 - Physical Chemistry IV

4 Credits

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, H_2 - Br_2 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 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), Tyndall effect; Electrokinetic phenomena (qualitative idea only); Determination of Avogadro number by Perrin's method; Stability of colloids and zeta potential; Micelle formation

Reference Books

- ▶ Castellan, G. W. Physical Chemistry, Narosa
- ▶ Levine, I. N. Physical Chemistry, Tata McGraw-Hill
- ▶ Atkins, P. W. & Paula, J. de Atkin's, Physical Chemistry, Oxford University Press
- ▶ McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
- ▶ Mortimer, R. G. Physical Chemistry, Elsevier
- ▶ Laidler, K. J. Chemical Kinetics, Pearson
- ▶ Banwell, C. N. Fundamentals of Molecular Spectroscopy, Tata-McGraw-Hill
- ▶ Barrow, G. M. Molecular Spectroscopy, McGraw-Hill
- ▶ Hollas, J.M. Modern Spectroscopy, Wiley India
- ▶ McHale, J. L. Molecular Spectroscopy, Pearson Education
- ▶ Wayne, C. E. & Wayne, R. P. Photochemistry, OUP
- ▶ Brown, J. M. Molecular Spectroscopy, OUP
- ▶ Levine, I. N. Quantum Chemistry, PHI
- ▶ Atkins, P. W. Molecular Quantum Mechanics, Oxford

2.28 Core P14 - Physical Chemistry IV Lab.

2 Credits

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.

3. Discipline Specific Electives Syllabus

3.1 DSE T1 – Advanced Physical Chemistry

4 Credits

Crystal Structure

1. Bravais Lattice and Laws of Crystallography: Types of solid, Bragg's law of diffraction; Laws of crystallography (Haüy's law and Steno's law); Permissible symmetry axes in crystals; Lattice, space lattice, unit cell, crystal planes, Bravais lattice. Packing of uniform hard sphere, close packed arrangements (fcc and hcp); Tetrahedral and octahedral voids. Void space in p-type, F-type and I-type cubic systems
2. Crystal planes: Distance between consecutive planes [cubic, tetragonal and orthorhombic lattices]; Indexing of planes, Miller indices; calculation of d_{hkl} ; Relation between molar mass and unit cell dimension for cubic system; Bragg's law (derivation)
3. Determination of crystal structure: Powder method; Structure of NaCl and KCl crystals

Statistical Thermodynamics

1. Configuration: Macrostates, microstates and configuration; calculation with harmonic oscillator; variation of W with E ; equilibrium configuration
2. Boltzmann distribution: Thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation); Applications to barometric distribution; Partition function, concept of ensemble - canonical ensemble and grand canonical ensembles
3. Partition function: molecular partition function and thermodynamic properties, Maxwell's speed distribution; Gibbs' paradox

Special selected topics

1. Specific heat of solid: Coefficient of thermal expansion, thermal compressibility of solids; Dulong –Petit's law; Perfect Crystal model, Einstein's theory – derivation from partition function, limitations; Debye's T^3 law – analysis at the two extremes
2. 3rd law: Absolute entropy, Plank's law, Calculation of entropy, Nernst heat theorem
3. Adiabatic demagnetization: Approach to zero Kelvin, adiabatic cooling, demagnetization, adiabatic demagnetization – involved curves
4. Polymers: Classification of polymers, nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers; Criteria for synthetic polymer formation; Relationships between functionality, extent of reaction and degree of polymerization; Mechanism and kinetics of step growth and copolymerization; Conducting polymers

Reference Books

- ▶ Castellan, G. W. Physical Chemistry, Narosa
- ▶ Levine, I. N. Physical Chemistry, Tata McGraw-Hill
- ▶ Moore, W. J. Physical Chemistry, Orient Longman
- ▶ Atkins, P. W. & Paula, J. de Atkins', Physical Chemistry, Oxford University Press
- ▶ McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
- ▶ Engel, T. & Reid, P. Physical Chemistry, Pearson
- ▶ Nash, L. K. Elements of Statistical Thermodynamics, Dover
- ▶ Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas
- ▶ Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata-McGraw-Hill
- ▶ Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
- ▶ Seymour, R. B. & Carraher, C. E. Polymer Chemistry: An Introduction, Marcel Dekker, Inc.
- ▶ Odian, G. Principles of Polymerization, Wiley
- ▶ Billmeyer, F. W. Textbook of Polymer Science, Wiley Interscience, 1971.

3.2 DSE P1 – Advanced Physical Chemistry Lab.

2 Credits

List of Practical

Computer Programming based on numerical methods for:

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

Reference Books

- ▶ McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008)
- ▶ Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005)
- ▶ Yates, P. Chemical Calculations. 2nd Ed. CRC Press (2007)
- ▶ Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007) Chapters 3-5
- ▶ Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985)

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 and special emphasis on the following:

1. Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products , Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions.
2. Prevention/ minimization of hazardous/ toxic products reducing toxicity. $\text{risk} = (\text{function}) \text{hazard} \times \text{exposure}$; waste or pollution prevention hierarchy.
3. Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorinated biphasic solvent, PEG, solventless processes, immobilized solvents and how to compare greenness of solvents.
4. Energy requirements for reactions – alternative sources of energy: use of microwaves and ultrasonic energy.
5. Selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups.
6. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis.
7. Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal Gas Tragedy (safer route to carbonyl) and Flixborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.
8. Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Examples of Green Synthesis/ Reactions and some real world cases

1. Green Synthesis of the following compounds: adipic acid, catechol, disodiumiminodiacetate (alternative to Strecker synthesis)
2. Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
3. Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

4. Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
5. Designing of Environmentally safe marine antifoulant.
6. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
7. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
8. Healthier Fats and oil by Green Chemistry: Enzymatic Inter esterification for production of no Trans-Fats and Oils
9. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

Future Trends in Green Chemistry

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

Reference Book

- ▶ Anastas, P.T. & Warner, J.K.: Green Chemistry - Theory and Practical, Oxford University Press (1998).
- ▶ Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
- ▶ Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
- ▶ Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
- ▶ Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.

3.4 DSE P2 – Green Chemistry Lab

2 Credits

Safer starting materials

1. Preparation and characterization of nanoparticles of gold using tea leaves.

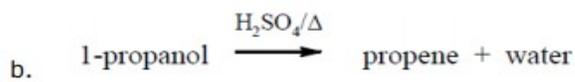
Using renewable resources

1. Preparation of biodiesel from vegetable/ waste cooking oil.

Avoiding waste

Principle of atom economy.

1. Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.
2. Preparation of propene by two methods can be studied
 - a. Triethylamine ion + OH⁻ → propene + trimethylpropene + water



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

Use of enzymes as catalysts

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

Alternative Green solvents

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

Mechanochemical solvent free synthesis of azomethines

Alternative sources of energy

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

Reference Books

- ▶ Anastas, P.T & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
- ▶ Kirchoff, M. & Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
- ▶ Ryan, M.A. Introduction to Green Chemistry, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
- ▶ Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN 978-93-81141-55-7 (2013).
- ▶ Cann, M.C. & Connelly, M. E. Real world cases in Green Chemistry, American Chemical Society (2008).
- ▶ Cann, M. C. & Thomas, P. Real world cases in Green Chemistry, American Chemical Society (2008).
- ▶ Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.
- ▶ Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach, W.B.Saunders, 1995.

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

1. Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.
2. UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;
3. 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.
4. 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.
5. Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, and 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 pKa values.

Separation techniques

1. Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation.
2. Technique of extraction: batch, continuous and counter current extractions.

3. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.
4. Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange.
5. Development of chromatograms: frontal, elution and displacement methods.
6. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.
7. 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).
8. Role of computers in instrumental methods of analysis.

Reference Books

- ▶ Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
- ▶ Willard, H.H. Et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- ▶ Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- ▶ Harris, D.C.: Exploring Chemical Analysis, 9th Ed. New York, W.H. Freeman, 2016.
- ▶ Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age International Publisher, 2009.
- ▶ Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
- ▶ Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
- ▶ Ditts, R.V. Analytical Chemistry; Methods of separation, van Nostrand, 1974.

3.6 DSE P3 – Analytical Methods of Chemistry Lab.

Credits

Separation Techniques – Chromatography

1. Separation of mixtures
Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.
2. Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.
3. Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

Solvent Extractions

1. 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.
2. Analysis of soil:

- a. Determination of pH of soil.
- b. Total soluble salt
- c. Estimation of calcium, magnesium, phosphate, nitrate
3. Ion exchange:
 - Determination of exchange capacity of cation exchange resins and anion exchange resins.

Spectrophotometry

1. Determination of pKa values of indicator using spectrophotometry
2. Determination of chemical oxygen demand (COD)
3. Determination of Biological oxygen demand (BOD)

Reference Books

- ▶ Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
- ▶ Willard, H.H. Et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- ▶ Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- ▶ Harris, D.C. Exploring Chemical Analysis, 9th Ed. New York, W.H. Freeman, 2016.
- ▶ Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age International Publisher, 2009.
- ▶ Skoog, D.A. Holler F.J. And Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Edition.
- ▶ Mikes, O. & Chalmes, R.A. Laboratory Handbook of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- ▶ Ditts, R.V. Analytical Chemistry: Methods of separation. Van Nostrand, New York, 1974.

3.7 DSE T4 – Polymer Chemistry

4 Credits

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 Polymer

(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 Book

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

3.8 DSE P4 – Polymer Chemistry Lab

2Credits

Polymer Synthesis

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

Polymer characterization

1. Determination of molecular weight by viscometry:
 - a. Polyacrylamide-aq.NaNO₂solution
 - 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

Reference Books

- ▶ M.P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed., Oxford University Press, 1999.
- ▶ H.R. Allcock, F.W. Lampe & J.E. Mark, Contemporary Polymer Chemistry, 3rd ed. PrenticeHall (2003)
- ▶ F.W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- ▶ J.R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
- ▶ P. Munk & T.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)
- ▶ M.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).

4.Skill Enhancement Subjects Syllabus

4.1 SEC T1 – Basic Analytical Chemistry

2 Credits

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

1. Determination of pH of soil samples.
2. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

Analysis of water

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

1. Determination of pH, acidity and alkalinity of a water sample.

2. Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products

Nutritional value of foods, idea about food processing and food preservations and adulteration.

1. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
2. Analysis of preservatives and colouring matter.

Chromatography

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

1. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).
2. To compare paint samples by TLC method.

Ion-exchange

1. Column, ion-exchange chromatography etc.
2. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Analysis of cosmetics

Major and minor constituents and their function

1. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
2. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration

Suggested Applications (Any one)

1. To study the use of phenolphthalein in trap cases.
2. To analyse arson accelerants.
3. To carry out analysis of gasoline.

Suggested Instrumental demonstrations

1. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flamephotometry.
2. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.
3. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drinks

Reference Books

- ▶ Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7thEd. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- ▶ Skoog, D.A., Holler, F.J. & Crouch, S. Principles of Instrumental Analysis, Cengage Learning India Edition, 2007.
- ▶ Skoog, D.A.; West, D.M. & Holler, F.J. Analytical Chemistry: An Introduction 6th Ed., Saunders College Publishing, Fort Worth, Philadelphia (1994).
- ▶ Harris, D. C. Quantitative Chemical Analysis, 9th ed. Macmillan Education, 2016.
- ▶ Dean, J. A. Analytical Chemistry Handbook, McGraw Hill, 2004.
- ▶ Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India, 1992.
- ▶ Freifelder, D.M. Physical Biochemistry 2nd Ed., W.H. Freeman & Co., N.Y. USA (1982).
- ▶ Cooper, T.G. The Tools of Biochemistry, John Wiley & Sons, N.Y. USA. 16 (1977).
- ▶ Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall, 1996.
- ▶ Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.
- ▶ Robinson, J.W. Undergraduate Instrumental Analysis 5th Ed., Marcel Dekker, Inc., New York (1995).
- ▶ Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.

4.2 SEC T2 – Pharmaceuticals Chemistry

2 Credits

Drugs & Pharmaceuticals

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

Fermentation

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

Hands On Practical

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.

5. Generic Electives Subjects Syllabus

5.1 GE T1 – Atomic Structure, Chemical Periodicity, Acids and Bases, Redox Reactions, General Organic Chemistry & Aliphatic Hydrocarbons 4 Credits

Inorganic Chemistry

1. 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.

2. 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.

3. 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.

4. Redox reactions

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

Organic Chemistry

1. 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.

2. 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.

3. Nucleophilic Substitution and Elimination Reactions

Nucleophilic substitutions: S_N1 and S_N2 reactions; eliminations: E1 and E2 reactions (elementary mechanistic aspects); Saytzeff and Hofmann eliminations; elimination vs substitution.

4. Aliphatic Hydrocarbons

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

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

6. Alkenes: (up to 5 Carbons). Preparation: elimination reactions: dehydration of alcohols and dehydrohalogenation of alkyl halides; cis alkenes (partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alkaline KMnO_4) 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.

7. Alkynes: (up to 5 Carbons). Preparation: acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal dihalides.

8. Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO_4 , ozonolysis and oxidation with hot alkaline KMnO_4 .

Reference Books

- ▶ Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- ▶ Cotton, F.A., Wilkinson, G. & Gaus, P.L. Basic Inorganic Chemistry, 3rd ed., Wiley.
- ▶ Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons.
- ▶ Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education Ind
- ▶ Sethi, A. Conceptual Organic Chemistry; New Age International Publisher.
- ▶ Parmar, V. S.A Text Book of Organic Chemistry, S. Chand & Sons.
- ▶ Madan, R. L. Organic Chemistry, S. Chand & Sons.
- ▶ Wade, L. G., Singh, M. S., Organic Chemistry.
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
- ▶ Sen Gupta, Subrata. Basic Stereochemistry of Organic molecules.
- ▶ Kalsi, P. S. Stereochemistry Conformation and Mechanism, Eighth edition, New Age International, 2014.
- ▶ Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.

5.2 GE P1 – Atomic Structure, Chemical Periodicity, Acids and Bases, Redox Reactions, General Organic Chemistry & Aliphatic Hydrocarbons Lab. 2 Credits

Inorganic Chemistry

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 $\text{Na}_2\text{S}_2\text{O}_3$.

Organic Chemistry

Qualitative Analysis of Single Solid Organic Compound(s)

1. Detection of special elements (N, Cl, and S) in organic compounds.
 2. Solubility and Classification (solvents: H_2O , dil. HCl, dil. NaOH)
 3. Detection of functional groups: Aromatic- NO_2 , Aromatic $-\text{NH}_2$, $-\text{COOH}$, carbonyl (no distinction of $-\text{CHO}$ and $>\text{C}=\text{O}$ needed), $-\text{OH}$ (phenolic) in solid organic compounds.
- Experiments 1 to 3 with unknown (at least 6) solid samples containing not more than two of the above type of functional groups should be done.

Reference Books

- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta, 2003.
- ▶ Das, S. C., Chakraborty, S. B., Practical Chemistry.
- ▶ Mukherjee, K. S. Text book on Practical Chemistry, New Oriental Book Agency.
- ▶ Ghosal, Mahapatra & Nad, An Advanced course in practical Chemistry, New Central Book Agency
- ▶ Vogel, A. I. Elementary Practical Organic Chemistry, Part 2: Qualitative Organic Analysis, CBS Publishers and Distributors.
- ▶ Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
- ▶ Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.

5.3 GE T2 – States of Matter & Chemical Kinetics, Chemical Bonding & Molecular Structure, P-Block Elements Credits

Physical Chemistry

1. Kinetic Theory of Gases and Real gases
 - a. 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
 - b. 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

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

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

2. Liquids

a. 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)

3. Solids

a. Forms of solids, crystal systems, unit cells, Bravais lattice types, Symmetry elements; Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices; Miller indices of different planes and interplanar distance, Bragg's law; Structures of NaCl, KCl and CsCl (qualitative treatment only); Defects in crystals; Glasses and liquid crystals.

4. Chemical Kinetics

a. 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

b. Temperature dependence of rate constant; Arrhenius equation, energy of activation; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

Inorganic Chemistry

1. Chemical Bonding and Molecular Structure

a. 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.

b. 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.

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

d. 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.

2. Comparative study of p-block elements
 - a. 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

- ▶ Barrow, G.M. Physical Chemistry Tata McGraw-Hill (2007).
- ▶ Castellan, G.W. Physical Chemistry 4th Ed. Narosa (2004).
- ▶ Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
- ▶ Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998).
- ▶ Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
- ▶ Chugh, K.L., Agnish, S.L. A Text Book of Physical Chemistry Kalyani Publishers
- ▶ Bahl, B.S., Bahl, A., Tuli, G.D., Essentials of Physical Chemistry S. Chand & Co. Ltd.
- ▶ Palit, S. R., Elementary Physical Chemistry Book Syndicate Pvt. Ltd.
- ▶ Mandal, A. K. Degree Physical and General Chemistry Sarat Book House
- ▶ Pahari, S., Physical Chemistry New Central Book Agency
- ▶ Pahari, S., Pahari, D., Problems in Physical Chemistry New Central Book Agency
- ▶ Cotton, F.A. & Wilkinson, G. Basic Inorganic Chemistry, Wiley.
- ▶ Shriver, D.F. & Atkins, P.W. Inorganic Chemistry, Oxford University Press.
- ▶ Wulfsberg, G. Inorganic Chemistry, Viva Books Pvt. Ltd.
- ▶ Rodgers, G.E. Inorganic & Solid State Chemistry, Cengage Learning India Ltd., 2008.

5.4 GE P2: States of Matter & Chemical Kinetics, Chemical Bonding & Molecular Structure, P-Block Elements Lab.

Si2 Credits

Physical Chemistry

1. 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
2. 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
3. Study the kinetics of the following reactions
 - a. Initial rate method: Iodide-persulphate reaction

- b. Integrated rate method:
- Acid hydrolysis of methyl acetate with hydrochloric acid
 - Compare the strengths of HCl and H₂SO₄ by studying kinetics of hydrolysis of methyl acetate

Inorganic Chemistry

Qualitative semi-micro 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

- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta, 2003.
- ▶ Palit, S.R., Practical Physical Chemistry Science Book Agency
- ▶ Mukherjee, N.G., Selected Experiments in Physical Chemistry J. N. Ghose & Sons
- ▶ Dutta, S.K., Physical Chemistry Experiments Bharati Book Stall
- ▶ Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
- ▶ Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011)

5.5 GE T3 – Chemical Energetics, Conductance, Organic Chemistry-II 4 Credits

Physical Chemistry

1. Chemical Energetics

a. 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

b. 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, Kirchoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

c. Statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine, refrigerator and efficiency; Entropy change of systems and surroundings for various processes and transformations; Auxiliary state functions (G and A) and Criteria for spontaneity and equilibrium.

2. Chemical Equilibrium:

a. Thermodynamic conditions for equilibrium, degree of advancement; 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 and relation among them; van't Hoff's reaction isotherm, 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.

3. Conductance

a. 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)

b. Transport Number and principles of Hittorf's and Moving-boundary method

Organic Chemistry

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

1. Aromatic Hydrocarbons

Benzene: Preparation: from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: electrophilic substitution (general mechanism); nitration (with mechanism), halogenations (chlorination and bromination), sulphonation and Friedel-Craft's reaction (alkylation and acylation) (up to 4 carbons on benzene); side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

2. Organometallic Compounds

Introduction; Grignard reagents: Preparations (from alkyl and aryl halide); concept of umpolung; Reformatsky reaction.

3. Aryl Halides

Preparation: (chloro-, bromo- and iodobenzene): from phenol, Sandmeyer reactions. Reactions (Chlorobenzene): nucleophilic aromatic substitution (replacement by $-OH$ group) and effect of nitro substituent (activated nucleophilic substitution).

4. Alcohols, Phenols and Ethers

a. Alcohols: (up to 5 Carbons). Preparation: 1° -, 2° - and 3° - alcohols: using Grignard reagent, reduction of aldehydes, ketones, carboxylic acid and esters; Reactions: With sodium, HX (Lucas test), oxidation (alkaline $KMnO_4$, acidic dichromate, concentrated HNO_3); Oppenauer oxidation;

b. Diols: Preparation (with OsO_4); pinacol- pinacolone rearrangement (with mechanism) (with symmetrical diols only).

c. Phenols: Preparation: cumene hydroperoxide method, from diazonium salts; acidic nature of phenols; Reactions: electrophilic substitution: nitration and halogenations; Reimer - Tiemann reaction, Houben-Hoesch condensation, Schotten -Baumann reaction, Fries rearrangement and Claisen rearrangement.

d. Ethers: Preparation: Williamson's ether synthesis; Reaction: cleavage of ethers with HI.

5. Carbonyl Compounds

Aldehydes and Ketones (aliphatic and aromatic): (Formaldehyde, acetaldehyde, acetone and benzaldehyde): Preparation: from acid chlorides, from nitriles and from Grignard reagents; general properties of aldehydes and ketones; Reactions: with HCN, ROH, NaHSO₃, NH₂-G derivatives and with Tollens' and Fehling's reagents; iodoform test; aldol condensation (with mechanism); Cannizzaro reaction (with mechanism), Wittig reaction, benzoin condensation; Clemmensen reduction, Wolff- Kishner reduction and Meerwein-Ponndorf- Verley (MPV) reduction.

Reference Books

- ▶ Barrow, G.M. Physical Chemistry Tata McGraw-Hill (2007).
- ▶ Castellan, G.W. Physical Chemistry 4th Ed. Narosa (2004).
- ▶ Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
- ▶ Mahan, B.H. University Chemistry 3rd Ed. Narosa (1998).
- ▶ Ekambaram, S. General Chemistry, Pearson.
- ▶ Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York (1985).
- ▶ Chugh, K.L., Agnish, S.L. A Text Book of Physical Chemistry Kalyani Publishers
- ▶ Bahl, B.S., Bahl, A., Tuli, G.D., Essentials of Physical Chemistry S. Chand & Co. Ltd.
- ▶ Palit, S. R., Elementary Physical Chemistry Book Syndicate Pvt. Ltd.
- ▶ Mandal, A. K. Degree Physical and General Chemistry Sarat Book House
- ▶ Pahari, S., Physical Chemistry New Central Book Agency
- ▶ Pahari, S., Pahari, D., Problems in Physical Chemistry New Central Book Agency
- ▶ Sethi, A. Conceptual Organic Chemistry; New Age International Publisher.
- ▶ Parmar, V. S.A Text Book of Organic Chemistry, S. Chand & Sons.
- ▶ Madan, R. L. Organic Chemistry, S. Chand & Sons.
- ▶ Wade, L. G., Singh, M. S., Organic Chemistry, Pearson.
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.

5.6 GE P3 – Chemical Energetics, Conductance, Organic Chemistry II Lab. 2 Credits

Physical Chemistry

(Minimum five experiments to complete)

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide
3. Determination of enthalpy of ionization of acetic acid
4. Determination of enthalpy of hydration of copper sulphate

Conductance

- a. Determination of dissociation constant of a weak acid (cell constant, equivalent conductance are also determined)
- b. Perform the following conductometric titrations: (Any one)
 - i. Strong acid vs. strong base
 - ii. Weak acid vs. strong base

Organic Chemistry

Identification of a pure organic compound

1. Solid compounds: oxalic acid, tartaric acid, succinic acid, resorcinol, urea, glucose, benzoic acid and salicylic acid.
2. Liquid Compounds: methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

Reference Books

- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta, 2003.
- ▶ Palit, S.R., Practical Physical Chemistry Science Book Agency
- ▶ Mukherjee, N.G., Selected Experiments in Physical Chemistry J. N. Ghose & Sons
- ▶ Dutta, S.K., Physical Chemistry Experiments Bharati Book Stall
- ▶ Bhattacharyya, R. C, A Manual of Practical Chemistry.
- ▶ Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
- ▶ Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.

5.7 GE T4: Transition Metal, Coordination Chemistry, Analytical and Industrial Chemistry; Functional Group Organic Chemistry 4 Credits.

Transition Elements (3d series)

- a. General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.
 - b. Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).
- ### 2. Coordination Chemistry
- a. Werner's coordination theory, Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6.
 - b. Drawbacks of VBT. IUPAC system of nomenclature .

Analytical and Industrial Chemistry

1. Error Analysis and Computer Applications

a. Error analysis: accuracy and precision of quantitative analysis, determinate, indeterminate, systematic and random errors; methods of least squares and standard deviations.

2. Industrial Chemistry

a. Fuels: classification of fuel; heating values; origin of coal, carbonization of coal, coal gas, producer gas, water gas, coal based chemicals; origin and composition of petroleum, petroleum refining, cracking, knocking, octane number, antiknock compounds, kerosene, liquefied petroleum gas (LPG), liquefied natural gas (LNG); petrochemicals (C1 to C3 compounds and their uses).

b. Fertilizers: manufacture of ammonia and ammonium salts, urea, superphosphate, biofertilizers.

c. Cement: portland cement: composition and setting of cement, white cement.

Organic Chemistry

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

1. Carboxylic Acids and Their Derivatives

a. Carboxylic acids (aliphatic and aromatic): strength of organic acids: comparative study with emphasis on factors affecting pK values; Preparation: acidic and alkaline hydrolysis of esters (B_{AC2} and A_{AC2} mechanisms only) and from Grignard reagents; Reactions: Hell - Vohlard - Zelinsky reaction and Claisen condensation; Perkin reaction.

b. Carboxylic acid derivatives (aliphatic): (up to 5 carbons). Preparation: acid chlorides, anhydrides, esters and amides from acids; Reactions: Comparative study of nucleophilicity of acyl derivatives; interconversion among acid derivatives.

2. Amines and Diazonium Salts

a. Amines (aliphatic and aromatic): strength of organic bases; Preparation: from alkyl halides, Gabriel's phthalimide synthesis, Hofmann degradation, by reduction of nitro compounds; Reactions: with HNO_2 (distinction of 1°, 2°- and 3°- amines), Schotten – Baumann reaction, Diazo coupling reaction (with mechanism).

b. Diazonium salts: Preparation: from aromatic amines; Reactions: conversion to benzene, phenol, benzoic acid and nitrobenzene.

c. Nitro compounds (aromatic): reduction under different conditions (acidic, neutral and alkaline).

3. Amino Acids and Carbohydrates

a. Amino Acids: Preparations (glycine and alanine only): Strecker synthesis, Gabriel's phthalimide synthesis; general properties; zwitterion, isoelectric point; ninhydrin reaction.

b. Carbohydrates: classification and general properties; glucose and fructose: constitution; osazone formation; oxidation-reduction reactions; epimers of glucose (definition and example only); cyclic structures of glucose (determination of ring-size excluded); ascending (Kiliani –Fischer method) and descending (Ruff's and Wohl's methods) in monosaccharides (aldoses only); mutarotation.

Reference Books

- ▶ Cotton, F.A. & Wilkinson, G. Basic Inorganic Chemistry, Wiley.
- ▶ Shriver, D.F. & Atkins, P.W. Inorganic Chemistry, Oxford University Press.
- ▶ Wulfsberg, G. Inorganic Chemistry, Viva Books Pvt. Ltd.
- ▶ Rodgers, G.E. Inorganic & Solid State Chemistry, Cengage Learning India Ltd., 2008.
- ▶ Gangopadhyay, P. K. Application Oriented Chemistry, Book Syndicate.
- ▶ Mondal, A. K & Mondal, S. Degree Applied Chemistry, Sreedhar Publications.
- ▶ Banerjee, S. P. A Text Book of Analytical Chemistry, The New Book Stall
- ▶ Sethi, A. Conceptual Organic Chemistry; New Age International Publisher.
- ▶ Parmar, V. S. A Text Book of Organic Chemistry, S. Chand & Sons.
- ▶ Madan, R. L. Organic Chemistry, S. Chand & Sons.
- ▶ Ekambaram, S. General Chemistry, Pearson.
- ▶ Wade, L. G., Singh, M. S., Organic Chemistry.
- ▶ Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- ▶ Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.
- ▶ Gangopadhyay, P. K. Application Oriented Chemistry, Book Syndicate.

5.8 GE P4 – Transition Metal, Coordination Chemistry, Analytical and Industrial Chemistry; Functional Group Organic Chemistry 2 Credits

Inorganic Chemistry

1. Complexometric estimation of metals ions:
Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
2. Preparation of any two of the following complexes and measurement of their conductivity:
 - a. tetraamminecarbonatocobalt (III) nitrate
 - b. tetraamminecopper (II) sulphate
 - c. potassium trioxalatoferrate (III) trihydrate
3. Compare the conductance of the complexes with that of M/1000 solution of NaCl , MgCl_2 and LiCl_3 .
Estimation of the total hardness of water sample by EDTA titration.

Organic Chemistry

1. The following reactions are to be performed, noting the yield of the crude product:
 - a. Nitration of aromatic compounds
 - b. Condensation reactions
 - c. Hydrolysis of amides/imides
 - d. Acetylation of aromatic amines
 - e. Benzoylation of aromatic amines
2. Purification of the crude product is to be made by crystallisation from water/alcohol.

Reference Books

- ▶ Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
- ▶ Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
- ▶ University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N. University of Calcutta, 2003.
- ▶ Das, S. C., Chakraborty, S. B., Practical Chemistry.
- ▶ Ghosal, Mahapatra & Nad, An Advanced Course in Practical Chemistry, New Central Book Agency.