Course Curriculum under

CHOICE BASED CREDIT SYSTEM

FOR

BACHELOR OF SCIENCE IN CHEMISTRY (HONOURS)

Department of Chemistry

ADAMAS UNIVERSITY

Barasat, Kolkata-700 126

Semester-I

Final Syllabus
Semester-I

Physical-I and Organic -IA (60 L) **(CHM11052)**

Unit 1: Kinetic theory of gases **(8)**

Concept of pressure and temperature. Nature of distribution of velocities in one, two and three dimensions. Maxwell's distribution of speeds. 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 $\geq \varepsilon$, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases. Basic idea about beta, gamma and error functions. 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. Viscosity of gas, temperature dependence of viscosity.

Unit 2: Liquid state **(7L)**

Nature of the liquid state, (short range order and long range disorder).Vapour Pressure. Surface tension, surface energy, excess pressure, capillary rise and measurement of surface tension. Work of cohesion and adhesion, spreading of liquid over surface. Vapor pressure over curved surface. Temperature dependence of surface tension.

Viscosity: Flows under the influence of mechanical, chemical and electrical forces: General features of fluid flow (streamline and turbulent flows, Reynold‘s number); nature of viscous drag for streamline motion, Newton‘s equation, viscosity coefficient, Poiseuille equation (with derivation), Viscosity of gas, temperature dependence of viscosity coefficient of liquid and comparison with that for gases; Stokes' law and terminal velocity; experimental determination of viscosity of liquids.

Unit 3: Thermodynamics I **(12L)**

Importance and scope, definition of system and surroundings: type of systems (isolated, closed and open); extensive and intensive properties; steady state versus equilibrium state; concept of thermal equilibrium and the zeroth law of thermodynamics; thermodynamic coordinates, state of a system, equation of state, state functions and path functions; partial derivatives and cyclic rule; concept of heat and work (IUPAC convention); graphical explanation of work done during expansion and compression of a ideal gas; reversible and irreversible processes and work done; first law of thermodynamics, internal energy (U) as a state function; enthalpy as a state function; energy conservation in the living organism; heat changes at constant volume and constant pressure; relation between C_p and C_v using ideal gas and van der Waals equations; joule‘s experiment and its consequence; explanation of term $(\delta U/\delta V)_T$; isothermal and adiabatic processes.

Thermo chemistry: heat changes during physicochemical processes at constant pressure/volume; Kirchhoff‘s relations; bond dissociation energies; changes of thermodynamic properties in different chemical changes.

Unit 4: An overview on Chemical kinetics (3L)

Differential rate law, idea of elementary and multistep reactions, order and molecularity. Arrhenius equation, energy of activation, reaction rate theory (only basics).

Reference Books:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford UniversityPress (2014).
2. Ball, D. W. *Physical Chemistry Thomson Pres*s, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
5. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).
6. Chatterjee, H. Physical Chemistry, Vol-1, 2nd Edition, Platinum publishers
7. Bera, N. Physical Chemistry, 1st Edition, Techno World Pub.

Organic -IA (30 L)

Unit 1: General Introduction and Bonding Features in Organic Molecules (12L)

Functional group based classification and nomenclature. Molecular formula and IHD / DBE.Valence bond theory: Concept of hybridisation, resonance (including hyperconjugation), inductive effect, steric effect, steric inhibition of resonance. Orbital pictures of bonding (sp^3, sp^2, sp: C-C, C-N & C-O system).

MO theory: Sketch and energy levels of MOs of i) acyclic π orbital system (C=C, conjugated diene and allyl systems) ii) cyclic π orbital system (neutral system: [4], [6] annulenes; charged system: 3, 4, 5-membered ring system); Frost diagram, Huckel's rules for aromaticity, antiaromaticity; homoaromaticity.

Physical properties: Melting point, boiling point; solubility; dipole moment; acid and base strength.

Unit 2: General treatment of reaction mechanism (8L)

Mechanistic classification: ionic, radical and pericyclic; heterolytic bond cleavage and heterogenic bond formation, homolytic bond cleavage and homogenic bond formation; representation of mechanistic steps using arrow formalism.

Reactive intermediates: carbocations (cabenium and carbonium ions), carbanions, carbon radicals, carbenes – structure using orbital picture, electrophilic/nucleophilic behaviour, stability, generation and fate (elementary idea)

Unit 3: Reaction thermodynamics & kinetics (10L)

Free energy and equilibrium, enthalpy and entropy factor, intermolecular &intramolecular reactions. Application of thermodynamic principles in tautomericequilibria [keto-enoltautomerism, composition of the equilibrium in different systems (simple carbonyl, 1,3 and 1,2- dicarbonyl systems, phenols and related system), substituent and solvent effect]. Concept of acids and bases: effect of structure, substituent and solvent on acidity and basicity. Reaction kinetics: transition state theory, rate const and free energy of activation, free energy profiles for one step and two step reactions, catalyzed reactions, kinetic control and

thermodynamic control of reactions, isotope effect, primary kinetic isotopic effect (kH/kD), principle of microscopic reversibility, Hammond postulate.

Reference Books:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
3. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry ofNatural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning IndiaEdition, 2013.
5. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).

Inorganic-I and Organic –IB (60 L) (CHM11053)

Inorganic-I (40L)

Unit-1: Extra nuclear Structure of atom (13L)

Bohr's theory, its limitations and atomic spectrum of hydrogen atom; Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and 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 rule of maximum spin multiplicity, Exchange energy, Aufbau principle and its limitations, Groundstate Term symbols of atoms and ions for atomic number up to 30.

Unit-2: Chemical periodicity (12L)

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

Unit-3: Theory of acids and bases (8L)

Acid-Base concept: Arrhenius concept, theory of solvent system (in H_2O, NH_3, $SO_2$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.Superacids, Gas phase acidity and proton affinity; HSAB principle.Acid-baseequilibria in aqueous solution, pH, buffer solutions and buffer actions, acid-base neutralization curves, acid-base indicators, choice of indicators, Acid-base titrations.

Unit-4: **Radioactivity** **(7L)**

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation.

References:

5. Douglas, B.E. and McDaniel, D.H. *Concepts & Models of Inorganic Chemistry* Oxford, 1970
6. Shriver and Atkins, *Inorganic chemistry*
7. Huheey, Keiter and Keiter, *Principles of Inorganic Chemistry*
8. R. Sarkar, Vol. 1 *Inorganic Chemistry.*
9. H. J Arnikar, *Nuclear chemistry..*

Organic IB (20L)

Stereochemistry-I **(20L)**

Representation of molecules in saw horse, Fischer, flying-wedge and Newman formulae and their inter translations, symmetry elements, molecular chirality.

Configuration: stereogenic units i) stereocentres: systems involving 1, 2, 3 centres, stereogenicity, chirotopicity. pseudoasymmetric (D/L and R/S descriptor, threo/erythro and syn/anti nomenclatures (for aldols) ii) stereoaxis: chiral axis in allenes& biphenyls, R/S descriptor; cis/trans, syn/anti, E/Z descriptors (for C=C, C=N). Optical activity of chiral compounds: specific rotation, optical purity (enantiomeric excess), racemic compounds, racemisation (through cationic and anionic and radical intermediates), resolution of acids, bases and alcohols via diastereomeric salt formation. Topicity of ligands and faces (elementary idea): Pro-R, Pro-S and Re /Si descriptors.

Conformation: Conformational nomenclature, eclipsed, staggered, gauche and anti; dihedral angle, torsion angle, energy barrier of rotation, relative stability of conformers on the basis of steric effect, dipole-dipole interaction, H-bonding; conformational analysis of ethane, propane, n-butane, haloethane, 1,2-haloethane, 1,2- glycol, 1,2-halohydrin; invertomerism of trialkylamines.Conformational analysis: 4, 5, 6-membered rings; mono- and di-substituted cyclohexane.

References:

1. Eliel, E. L. &Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London,1994.
2. Nassipuri, D. *Stereochemistry of organic compounds*
3. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, New Age International,2005.

Physical Lab I **(CHM12054)**

Surface tension measurements.

Lab 1. Determine the surface tension by (i) drop number (ii) drop weight method.
Lab 2. Study the variation of surface tension of detergent solutions with concentration.
Lab 3: Determination of CMC of a micelle from Surface Tension Measurement.

Viscosity Measurement:

Lab4: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water.
Lab5: Study of the variation of viscosity with the concentration of the solution.

Enthalpy determination:

Lab 6: Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
Lab 7: Determination of heat of neutralization of a strong acid by a strong base
Lab 8: Study of the solubility of benzoic acid in water and determination of ΔH.

References:

1. Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
2. Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
3. University Hand Book of Undergraduate Chemistry Experiments, University of Calcutta.
4. 1. Athawale, V. D. &Mathur, P. *Experimental Physical Chemistry* New AgeInternational: New Delhi (2001).

Inorganic Lab I **(CHM12055)**

Qualitative semimicro analysis of mixtures containing not more than three radicals.

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

Anion Radicals: F^-, Cl^-, Br^-, BrO_3^-, I^-, NO_3^-, SCN^-,S^{2-},SO_4^{2-}, NO_2^-, PO_4^{3-}, AsO_4^{3-},BO_3^{3-}, CrO_4^{2-} / $Cr_2O_7^{2-}$, $[Fe(CN)_6]^{4-}$, $[Fe(CN)_6]^{3-}$

References:

1. Vogel's Qualitative Inorganic Analysis (7th Edition): G. Svehla
2. Handbook of Inorganic Analysis (First Edition): U.N Dhur& Sons Private Ltd.

Semester-II

Organic -II and Physical IIA (60 L) **(CHM11056)**

Organic (50L)

Unit-1- Carbon-Carbon sigma bonds **(5 L)**

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

Nucleophilic substitution reactions **(20L)**

Substitution at sp^3 centre - Mechanism: SN1, SN2, SN2', SNi mechanisms, effect of solvent, substrate structure, leaving group, nucleophiles including ambident nucleophiles (cyanide & nitrite) substitution involving NGP; relative rate &stereochemical features [systems: alkyl halides, allyl halides, alcohols, ethers, epoxides; Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Unit-2-Carbon-Carbon pi bonds: (10L)

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cB reactions.Saytzeff and Hofmann eliminations, stereoselectivity; substitution vs elimination

Unit-3: Electrophilic addition to C=C: (15L)

Mechanism (Markownikoff/ Anti Markownikoff addition), reactivity, regioselectivity and stereoselectivity. Reactions: halogenations, hydrohalogenation, of oxymercuration-demercuration, hydroboration-oxidation,, hydrogenation, epoxidation, hydroxylation, ozonolysis, electrophiilic addition to diene (conjugated dienes and allenes), Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethylbenzene.

Radical addition: HBr addition.

Dissolving metal reduction of alkynes and bezenoid aromatics (Birch).Pericyclic addition: Diels-Alder reaction.

Addition of singlet and triplet carbenes.; Simmons-Smith reaction

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

References Books:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
3. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
4. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.

Physical IIA

Chemical Kinetics I (10L)

Phenomenological kinetics: degree of advancement of a reaction, reaction rate, rate constant, order and molecularity of a reaction, determination of order of a reaction by half-life and differential method: zero, first, second and fractional order reactions, pseudo first order reaction; solutions of elementary differential equations, complex reaction: opposing, parallel and consecutive reactions (all step of first order), kinetic and thermodynamic control of reaction; idea of rate determining step; steady-state approximation; kinetics and mechanism of

reaction; kinetics of chain reaction; temperature dependence of rate constant. Collision theory, Outline of transition state theory.

References:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. McQuarrie, D. A & Simon, J. D, Physical Chemistry: A molecular approach, University Science Books, Sausalito, California.
5. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
6. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Inorganic -II and Physical IIB (60L) (CHM11057)

Inorganic-II (30L)

Unit-1: Chemical Bonding (25 L)

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule andits application and limitations. Packing of ions in crystals.Born-Landé equation withderivation and importance of Kapustinskii expression for lattice energy.Madelungconstant, Born-Haber cycle and its application, Solvation energy.Defects in solids(elementary idea). Solubility energetics of dissolution process

(ii) *Covalent bond:* Polarizing power and polarizability, ionic potential, Fazan'srules.Lewis structures, formal charge. Valence Bond Theory. The hydrogen molecule(Heitler-London approach), directional character of covalent bonds, hybridizations,equivalent and non-equivalent hybrid orbitals, Bent's rule, Dipole moments, VSEPRtheory, shapes of molecules and ions containing lone pairs and bond pairs (examplesfrom main groups chemistry) and multiple bonding (σ and π bond approach).

(iii) Molecular orbital concept of bonding (The approximations of the theory, Linear combination of atomic orbitals (LCAO) (elementary pictorial approach): sigma and pibonds and delta interaction, multiple bonding. Orbital designations: *gerade*, *ungerade*, HOMO, LUMO. Orbital mixing,. MO diagrams of H_2, Li_2, Be_2, B_2, C_2, N_2, O_2, F_2, and their ions wherever possible; Heteronuclear molecular orbitals: CO, NO, NO^+, CN^-, HF, BeH_2, $CO_2$and H_2O. Bond properties: bond orders, bond lengths.

Unit-2: Noble Gases: (5L)

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparationand 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-oxygencompounds. Molecular shapes of noble gas compounds (VSEPR theory)

References:

1. 1.Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic ChemistryOxford, 1970

2. Shriver and Atkins, Inorganic chemistry
3. Huheey, Keiter and Keiter, Principles of Inorganic Chemistry
4. R. Sarkar, Vol. 1 Inorganic Chemistry
5. Greenwood and Esarnshaw, Chemistry of the elements
6. J. D. Lee, Concise Inorganic Chemistry
7.

Physical IIB (30L)

Unit 1: Thermodynamics II **(20L)**

Second law of thermodynamics: need for a second law, Clausius and Kelvin-Planck statements and their equivalence; Carnot's theorem, thermodynamic scale of temperature, concept of heat engine, Carnot cycle and refrigerator; Clausius inequality, entropy as a state function, second law in terms of entropy, calculation of entropy change for various transformation; auxiliary state function (G and A) and their variation with temperature, pressure and volume; criteria of spontaneity and equilibrium; Gibbs-Helmholtz equation; Maxwell's relation, thermodynamic equation of state, C_p-C_v values, Joule-Thomson co-efficient for van der Waal's gases.
Open system, chemical potential and activity, partial molar quantities, chemical potential in terms of Gibbs free energy and other thermodynamic state functions and its variation with temperature and pressure, Gibbs-Duhem equation; Euler's theorem; expression for ideal gas.
Non-ideal system: idea of fugacity and activity; standard states.

Unit 2: Real gas **(10L)**

Deviation of gases from ideal behaviour (compressibility factor, Andrew's and Amagat's plots); van der Waals equation of state: derivation and characteristic features; existence of critical state; critical constants in terms of van der Waals constants, the law of corresponding states; virial equation of state and significance of the second virial co-efficient, Boyle temperature, the Dieterici equation of state (preliminary ideas only); intermolecular forces and potentials (Keesom, Debye and London).

References:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. McQuarrie, D. A & Simon, J. D, Physical Chemistry: A molecular approach, University Science Books, Sausalito, California.
5. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
6. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).

Physical Lab II **(CHM12063)**

<u>Kinetics Measurement by titrimetric method:</u>

Lab1: Study of kinetics of decomposition of H_2O_2.

Lab2: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate.

Polarimeter

Lab 3: Determination of specific rotation of optically active compound.
Lab 4: Inversion of can-sugar.

Refractive index:

Lab 5: Determination of composition of a binary mixture by refractive index study.

References:

1. Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
2. Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
3. University Hand Book of Undergraduate Chemistry Experiments, University of Calcutta.

Organic Lab I (CHM12059)

Organic Qualitative: Detection of elements and functional groups, detection of some single compounds

A. Detection of special elements (N, Cl, S) by Lassaigne's test
B. Solubility and Classification (solvents: H_2O, 5% HCl, 5% $NaHCO_3$, 5% NaOH)
C. Detection of the following functional groups by systematic chemical tests:
Aromatic amino ($-NH_2$), aromatic nitro ($-NO_2$), Amido ($-CONH_2$, including imide),Phenolic –OH, Carboxylic acid (-COOH), Carbonyl (>C=O); only one test for each functional group is to be reported. Organic compounds.

Reference Books

- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education(2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012).
- Das, S.C. Advanced Practical Chemistry, Sixth edition

SEMESTER III

Physical III (60 Lectures) (CHM11060)

Unit 1 – Chemical Equilibrium and Ionic Equilibrium (20L)

Chemical Equilibrium: Thermo dynamics and equilibrium, degree of advancement, vant-Hoff's reaction isotherm (deduction from chemical potential), equilibrium constant and standard Gibbs free energy change; definition of K_p, K_c, K_x; vant Hoff's reaction isobar and isochore from different standard states; shifting of equilibrium due to change of external parameters like temperature and pressure and influence of inert gas; Le Chatelier principle of

dynamic equilibrium (thermodynamics approach) and its application to homogeneous chemical equilibria.
Nernst's distribution law; Application
Ionic equilibrium: concept of pH, hydrolysis of salts, buffer solution, elementary idea of biological buffers, acid-base indicators; solubility equilibria and influence of common and indifferent ions there on.

Unit-2- Chemical Kinetics-II (10L)

Lindeman theory of unimolecular reaction; primary kinetic salt effect. Catalysed reactions: homogeneous catalysis, mechanism of catalytic action, acid-base catalysis, auto catalysis, enzyme catalysis - kinetics and various kinds of inhibition: Michaelis-Menten equation, turnover number, Lineweaver-Burk plot; influence of temperature and pH

Unit 3 – Transport phenomena and electrochemistry (15L)

Molecular motions in liquids, electrolytic conduction: Electronic versus electrolytic conduction, measurement of conductance, cell constant; specific, equivalent and molar conductance; variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions, ion conductance and ionic mobility; Walden's rule; equivalent conductance at infinite dilution and its determination for strong and weak electrolytes; Debye –Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ostwald dilution law and determination of ionization constants for weak electrolytes from conductance measurements; applications of conductance measurement: determination of solubility product and ionic product of water, conductometric titration; transport number, Hittorf's rule, determination of transport number by the moving boundary method.

Unit 4 - Colloid and Surface science (15L)

Lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, zeta potential and Stern double layer (qualitative idea); Tyndall effect, electrokinetic phenomenon (qualitative idea only).
Special features of interfaces compared to bulk, surface dynamics: physical and chemical adsorption, Freundlich and Langmuir adsorption isotherm, multilayer and BET isotherm (without derivation) and applications, Gibbs adsorption isotherm and surface excess, effect of addition of substances on surface tension, surfactants and micelles and reverse micelles: applications, size and solubility; Microencapsulation for personal care; Nanoencapsulation. Heterogeneous catalysis (single reactant).

References:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. McQuarrie, D. A & Simon, J. D, Physical Chemistry: A molecular approach, Viva student edition
5. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).

6. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).
7. Chatterjee, H. Physical Chemistry, Vol-1&3 2nd Edition, Platinum publishers.

Inorganic III (60L) (CHM11061)

Unit-1: Chemistry of *s* and *p* Block Elements (30 L)

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

Unit-2: Redox reactions and precipitation equilibria in solution (30 L)

Ion-electron method of balancing equation of redox reaction.Elementary idea onstandard redox potentials with sign conventions, Nernst equation (without derivation).Influence of complex formation, precipitation and change of pH on redox potentials; formalpotential.Feasibility of a redox titration, redox potential at the equivalence point, redox titrations, 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 theprecipitation and separation of common metallic ions as hydroxides, sulfides,phosphates, carbonates, sulfates and halides.

References:

1. Shriver and Atkins, Inorganic chemistry
2. R. Sarkar, Vol. 1 Inorganic Chemistry
3. Greenwood and Esarnshaw, Chemistry of the elements
4. Gary L. Miessler, Paul J. Fischer, Donald A. Tarr. Inorganic Chemistry, 5th Edition.

Organic III (60L) (CHM11062)

Unit-1-Electrophilic aromatic substitution: (15 L)

Mechanisms, orientation and reactivity. Reactions: nitration, nitrosation, sulfonation, halogenation, Friedel-Crafts reactions, onecarbonelectrophiles (reactions: chloromethylation, Gatterman-Koch, Gatterman, Hoesch, Vilsmeier-Haack reaction, Reimer-Tiemann, Kolbe-Schmidt). Nucleophilic aromatic substitution: Addition-elimination mechanism, SN1 mechanism, benzyne mechanism.
Radical substitution: aromatic system.

Unit 2: Introduction to Alcohols: (5L)

Classification and nomenclature, Monohydric alcohols-nomenclature, methods of formation by reduction from aldehydes, ketones, carboxylic acids and esters. Hydrogen bonding, acidic nature. Reactions of alcohols, Dihydric alcohols-nomenclature, methods of formation, chemical reaction of vicinal glycols, oxidative cleavage (Pb(OAc)2 and HIO4), pinacol-pinacolone rearrangement, Trihydric alcohols-nomenclature and method of formation, chemical reaction of glycerols.

Unit-3: Synthesis of carbonyl compounds &Nucleophilic addition to C=O (30L)

Synthesis from alcohols, alkenes and alkynes and reactions: Mechanism, reactivity, equilibrium and kineticcontrol.Reactions with alcohols, amines, thiols, HCN, bisulfate, Wittig reaction.

Carbonyl Reduction: hydride addition, Wolff-Kishner reduction, dissolving metal(Bouveault-Blanc reduction), Clemmensen Reduction, reduction with metal hydrides

Characteristic reactions: Cannizzaro reaction, Tischenkoreaction, aldol condensation, benzoin condensation, Darzensreaction,Acyloin Condensation, Mannich reaction, Wittig reaction, Halogenation, Benzillic acid rearrangement, oxidation reactions (chromic acid oxidation, Riley oxidation), Perkin Reaction, Stobbe condensation, Knoevenagel condensation. Nucleophilic addition to α,β-unsaturated carbonyl system (general principles). Michael addition, Robinson annulation

Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Unit-4: Carboxylic Acids and their Derivatives: (10L)

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

Preparation and reactions of acid chlorides, anhydrides, esters and amides;

Substitution at sp^2 carbon (carbonyl system) - Comparative study of nucleophilic substitution at acyl group -Mechanism: BAC2, AAC2, AAC1, AAL1 (in connection to acid and ester). Systems: amides, anhydrides & acyl halides [formation and hydrolysis]Hydrolysis of nitriles and isonitriles.

Reference Books:

1. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
2. Norman &Coxon Principles of Organic Synthesis (CRC Press)
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
5. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, OxfordUniversity Press.
6. J. March,*Advanced Organic Chemistry*.

Physical Lab III: (CHM12069)

Buffer solution:

Lab1: Find out the pH of an unknown solution by colour matching method.

pH metry:

Lab 2: Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.

Lab 3: pH metric titration of i)strong acid vs. strong base ii) weak acid vs. strong base

Solubility product:

Lab 4: Determination of solubility product for sparingly soluble salt.

Partition Coefficient:

Lab 5: Determination of partition coefficient of iodine between water and organic solvent.

Adsorption

Lab 6: Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

References:

1. Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
2. Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
3. University Hand Book of Undergraduate Chemistry Experiments, University of Calcutta.

Organic Lab II (CHM12064)

A. Organic preparations:

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

1. Nitration of aromatic compounds
2. Hydrolysis of amides/ imides/ esters
4. Acetylation of phenols / aromatic amines (using conventional and green approach)
5. Benzoylation of phenols / aromatic amines
6. Side chain oxidation of aromatic compounds
7. Diazo coupling reactions of aromatic amines
9. Redox reaction; Oxidation of ethanol/ isopropanol (Iodoform reaction)..
10. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

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

C. MP of the purified product is to be noted.

Reference Books

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education(2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical OrganicChemistry, 5th Ed.*, Pearson (2012).
3. Das, S.C. *Advanced Practical Chemistry*, Sixth edition
4. Mukherjee, G.N. *University handbook of undergraduate chemistry experiments*

Inorganic Lab II **(CHM12058)**

(further details will be provided during the course)

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.

Oxidation-Reduction Titrations:

1. Estimation of Fe(III) and Mn(II) in a mixture using standardized $KMnO_4$solution
2. Estimation of Fe(III) and Cr(III) in a mixture using $K_2Cr_2O_7$.

Iodometry:

1. Estimation of Cu(II) by standardized sodium thiosulphate solution.
2. Estimation of Zn(II)by standardized sodium thiosulphate solution.
3. Estimation of Fe(III) and Cu(II) in a mixture.

References:

1. Subhas C Das, *Advanced Practical Chemistry*.
2. Handbook of Inorganic Analysis (First Edition): U.N Dhur& Sons Private Ltd.
3. An Advanced Course in *Practical*Chemistry ,Nad, *Mahapatra&Ghosal.*

Skill Enhancement Course (SEC)

SEC: Intellectual Property Rights (30 L) **(CHM11015)**

Unit 1: IPR Theory

In this era of liberalization and globalization, the perception about science and its practices has undergone dramatic change. The importance of protecting the scientific discoveries, with commercial potential or the intellectual property rights is being discussed at all levels –

statutory, administrative, and judicial. With India ratifying the WTO agreement, it has become obligatory on its part to follow a minimum acceptable standard for protection and enforcement of intellectual property rights. The purpose of this course is to apprise the students about the multifaceted dimensions of this issue.
Introduction to Intellectual Property:
Historical Perspective, Different Types of IP, Importance of protecting IP.

Unit 2: Copyrights
Introduction, How to obtain, Differences from Patents.

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

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

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

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

Layout design of integrated circuits
Circuit Boards, Integrated Chips, Importance for electronic industry.

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

Different International agreements
(a) Word Trade Organization (WTO):
(i) General Agreement on Tariffs & Trade (GATT), Trade
Related Intellectual Property Rights (TRIPS) agreement
(ii) General Agreement on Trade related Services (GATS)
(iii) Madrid Protocol
(iv) Berne Convention
(v) Budapest Treaty
(b) Paris Convention
WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

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

Reference Books:

- N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).
- Manjula Guru &*M.B.* Rao, *Understanding Trips: Managing Knowledge inDeveloping Countries*, Sage Publications (2003).
- P. Ganguli, Intellectual Property Rights: *Unleashing the Knowledge Economy*, TataMcGraw-Hill (2001).

Or

SEC: Chemistry of Cosmetics & Perfumes (30 L) (CHM11025)

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

Practicals

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

Reference Books:

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

Or

SEC: Fuel Chemistry (30L) (CHM11017)

Review of energy sources (renewable and non-renewable): Classification of fuels and theircalorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal.Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications. Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels.

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.
Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Reference Books:

1. Stocchi, E. *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK (1990).
2. Jain, P.C. & Jain, M. *Engineering Chemistry* DhanpatRai& Sons, Delhi.
3. Sharma, B.K. & Gaur, H. *Industrial Chemistry*, Goel Publishing House, Meerut(1996).

Semester –IV

Physical IV **(CHM11066)**

Unit-1: Quantum Mechanics-1 **(30L)**

Beginning of quantum mechanics: Black body radiation, wave-particle duality, light as particle, Photoelectric effect, Compton effect (without derivation), electrons as waves and the de Broglie hypothesis, Uncertainty principle.

Concept of operator and wave function: Time-independent form of the Schrödinger equation; probabilistic interpretation of the wave function; conditions for acceptability of wave functions; elementary idea of operator, operator algebra, eigen value equation, expectation value; time dependent Schrödinger equation, concept of stationary states, study of a simple (model) system:

Particle in box: Particle in a box problem: setting up of the Schrödinger equation, its solution, interpretation of the solutions (in the light of energies and wave functions) – normalization, orthogonality and probability eigenfunctions and eigenvalues, energy quantization (and its connection to the boundary conditions), evaluation of expectation values of x, x^2, p_x, p_x^2, their significance in the light of uncertainty principle, extension of the particle in one-dimensional box to two- and three- dimensional cases, idea of degenerate energy states and relationship of symmetry and degeneracy. Free particle.

Simple harmonic oscillator (SHO): setting up of the Schrödinger equation, connection with the uncertainty principle, classical turning points, expressions for energy and wave functions for the ground and the first excited states (quantitative treatment), series solutions of differential equation: Hermite equation, their characteristics features, the zero-point energy and its importance, limitations thereof and the idea of the anharmonic oscillator.

Unit-2: Colligative properties **(5)**

ΔG, ΔS, ΔH and ΔV of mixing for binary solutions, vapour pressure of solution, ideal solutions, ideally dilute solutions and colligative properties, Raoult‘s law, thermodynamic derivation (using chemical potentials) of colligative properties of solution and their inter-relationships, abnormal colligative properties, van‘t Hoff factor; biomedical application: osmosis and dialysis.

Unit 2 - Phase rule **(12L)**

Definition of phase, number of component and degrees of freedom, Gibbs phase rule and its derivation, definition of phase diagram, phase equilibria for one component system, first order phase transition and Clapeyron equation , Clausius-Clapeyron equation: derivation and its use; liquid vapor equilibrium for two component systems, Phenol-water system. Three component systems, water-chloroform-acetic acid system, triangular plots.

Ideal solution at a fixed temperature and pressure, principle of fractional distillation, Duhem-Margules equation, Henry's law, Konowaloff's rule; positive and negative deviations from ideal behaviour, azeotropic solutions, liquid-liquid phase diagram using phenol-water system, solid-liquid phase diagram, simple eutectic diagram.

Unit 4 - Thermodynamics Application in Electrochemistry (13L)

Types of electrochemical cells and examples, cell reactions, EMF and changes in free energy, ΔH and ΔS of cell reactions from EMF measurements; thermodynamic derivation of Nernst equation, standard cells, half cells/electrodes, different types of electrode (with examples), standard electrode potential (IUPAC convention) and principle of its determination; types of concentration cells, liquid junction potential and its minimization, determination of transport number by EMF method, glass electrode and determination of pH, applications of EMF measurement: potentiometric titrations: acid-base, redox and precipitation. Activity coefficient of electrolytes/ions in solution, Debye-Hückel model: limiting law, applications.

References:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. McQuarrie, D. A & Simon, J. D, Physical Chemistry: A molecular approach, Viva student edition
5. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
6. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).
7. Chatterjee, H. Physical Chemistry, Vol-2, 2nd Edition, Platinum publishers.

Inorganic IV (CHM11067)

Unit-1: Coordination Chemistry-I (15 L)

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.

Unit-2: Coordination Chemistry-II (30 L)

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 dions and their correlation with effective magnetic moments, including orbital contribution; quenching of

magnetic moment: superexchange 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 ofligands; charge transfer spectra (elementary idea).

Unit-3: Chemistry of d- and f- block elements (15 L)

General comparison of 3d, 4d and 5d elements in term of electronic configuration, elemental forms, metallic nature, atomization energy, oxidation states, redox properties, coordination chemistry, spectral and magnetic properties. f-block elements: electronic configuration, ionization energies, oxidation states, variation in atomic and ionic (3+) radii, magnetic and spectral properties of lanthanides, comparison between lanthanide and actinides.

References:

1. Shriver and Atkins, *Inorganic chemistry*
2. Huheey, Keiter and Keiter, *Principles of Inorganic Chemistry*
3. R. Sarkar, Vol. 2 *Inorganic Chemistry*
4. D. M. P. Mingos, Essential Trends in Inorganic Chemistry

Organic IV (60 Lectures) (CHM11068)

Unit 1 Nitrogen compounds and Organometallics (10 L)

Nitrogen compounds: amines (aliphatic & aromatic) [preparation, separation and identification of primary, secondary and tertiary amines], E. Clarke reaction, chemistry of enamines, diazomethane, diazoacetic ester, aromatic nitro compounds, aromatic diazonium salts, nitrile and isonitrile.

Organometallics: preparation of Grignard reagent and organo lithium. Reactions: addition of Grignard and organo lithium to carbonyl compounds, substitution on -COX, conjugate addition by Gilman cuprates, Reformatsky reaction.

Unit 2 Reactions: Rearrangements (20L)

Rearrangement to electron-deficient carbon (Wagner-Meerwein rearrangement, pinacol rearrangement, dienone-phenol; Wolff rearrangement in Arndt- Eistert synthesis, benzil-benzilic acid rearrangement). Electron-deficient nitrogen (Beckmann rearrangement, Schmidt rearrangement, Hofmann rearrangement, Lossen rearrangement, Curtius rearrangement). Electron-deficient oxygen (Baeyer-Villiger oxidation, hydroperoxide rearrangement (cumenehydroperoxide-phenol rearrangement), Dakin reaction. Aromatic rearrangements [migration from oxygen to ring carbon (Fries rearrangement, Claisen rearrangement, dienone-phenol rearrangement); migration from nitrogen to ring carbon (Hofmann-Martius rearrangement, Fischer-Hepp rearrangement, N-azo to C-azo rearrangement, Bamberger rearrangement, Orton rearrangement, benzidine rearrangement. **Transformation:** Radical coupling (pinacol, acyloin, McMurry), epoxides, phenols and quinones

Unit-3: Carbocycles and heterocycles (30L)

Carbocycles (10L): *Synthesis and reactions:* Thermodynamic and kinetic factors, Baldwin rules. Synthesis of carbocycles through alkylation, condensation, cycloaddition, rearrangement

and their reactions. Synthesis of polycyclic aromatics- of naphthalene, anthracene and phenanthrene.

Heterocycles (20L): Classification and nomenclature**;** Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom Synthesis and reactions of heterocycles (monocyclic and bicyclic) with one heteroatom-: reactivity, orientation and important reactions of furan, pyrrole, pyridine, indole, synthesis (including retrosynthetic approach) pyrrole: Paal-Knorr, Knorr pyrrole synthesis and Hantzsch synthesis. Hantzsch pyridine synthesis.Indole: Fischer-indole, Madelung and Reissert synthesis, Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander's synthesis, Knorr quinoline synthesis, Doebner-Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction**.** Derivatives of furan: Furfural and furoic acid, Quinoline and Quinazoline- syntheses, reactions, uses.

Reference Books:

1. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
2. Norman &Coxon Principles of Organic Synthesis (CRC Press)
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
5. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.
6. Joule and Mills, *Heterocyclic Chemistry*- 4th edition(Wiley)
7. Gilchrist, T.L. *Heterocyclic Chemistry* (Pearson).

Physical Lab IV **CHM12075**

Conductometric Experiment:

Lab 1: Conductometric titration of an acid (strong, weak/ monobasic, dibasic, and acid mixture) against strong base.

Lab 2: Study of saponification of ester conductometrically

Lab 3: Oswald dilution law

Lab4: Study the equilibrium of at least one of the following reactions by the distribution method:

(i) $I_2(aq) + I^-(aq) \rightarrow I_3^-(aq)$

(ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)_n$

Potentiometry

Lab 5 : Potentiometric titration of Mohr's salt solution against standard $K_2Cr_2O_7$ solution.

Lab 6 **:** Determination of K_{sp} for AgCl by potentiometric titration of $AgNO_3$ solution against standard KCl solution.

References:

1. Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
2. Levitt, B. P. edited Findlay's Practical Physical Chemistry Longman Group Ltd.
3. University Hand Book of Undergraduate Chemistry Experiments, University of Calcutta.

Organic Lab III (CHM12070)

Chromatography (Any one):

a. Introduction to thin layer chromatography (TLC).
b. Monitoring reaction progress by TLC.
c. Introduction to column chromatography.
d. Separation a mixture of two solid compounds by Column chromatography.
e. Separation a mixture of two liquid compounds by Column chromatography.

Reference text:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry,* Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)
3. Mukherjee, G.N. *University handbook of undergraduate chemistry experiments*
4. P.S. Kalsi, *Spectroscopy of organic compounds*

Inorganic Lab III (CHM12065)

(Further details will be provided during the course)

Iodometry:

1. Estimation of available chlorine in bleaching powder.
2. Estimation of strength of H_2O_2 sample by standardized sodium thiosulphate solution.

Complexometry:

1. Estimation of Ca(II) by EDTA complexometry.
2. Estimation of Ca(II) and Mg(II) in a given mixture.
3. Estimation of permanent and temporary hardness of water.
4. Estimation of nickel (II) using Dimethylglyoxime (DMG).

References:

1. Subhas C Das, *Advanced Practical Chemistry*.
2. Handbook of Inorganic Analysis (First Edition): U.N Dhur& Sons Private Ltd.
3. An Advanced Course in *Practical*Chemistry ,Nad, *Mahapatra*&*Ghosal.*

Skill enhancement course

SEC: Pharmaceutical Chemistry (30L) (CHM11016)

Drugs & cosmetics

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of therepresentative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam),Cardiovascular (Glyceryltrinitrate), antilaprosy (Dapsone), HIV-AIDS relateddrugs (AZT- Zidovudine), 7-Fluoroquinoline based drugs, Remdesivir, Tamiflu.

Fermentation

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

Practicals

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Or

SEC: Green Methods in Chemistry (30 L) (CHM11026)

Unit-1: Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry.Goals of Green Chemistry.Limitations/ Obstacles in the pursuit of the goals of Green Chemistry

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

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

a) 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.
b) Prevention/ minimization of hazardous/ toxic products reducing toxicity.risk = (function) hazard × exposure; waste or pollution prevention hierarchy.
c) Green solvents– supercritical fluids, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventlessprocesses, immobilized solvents and how to compare greenness of solvents.
d) Energy requirements for reactions – alternative sources of energy: use of microwavesand ultrasonic energy.
e) Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD “What you don’t have cannot harm you”, greener alternative to Bhopal

Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.

f) Strengthening/ development of analytical techniques to prevent and minimize thegeneration of hazardous substances in chemical processes.

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

a) Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis).
b) Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoicacid, oxidation of toluene and alcohols; microwave assisted reactions in organic solventsDiels-Alder reaction and Decarboxylation reaction.
c) Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonicalternative to Iodine).
d) A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
e) Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.
f) Environmentally safe antifoulant.
g) CO_2 as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
h) Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
i) A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
j) Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
k) Development of a fully recyclable carpet: cradle to cradle carpeting.

Reference Books:

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press.
2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole.
3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New.
4. Ahluwalia, V.K. &Kidwai, M.R.*New Trends in Green Chemistry*, AnamalayaPublishers (2005).
5. Anastas, P.T. & Warner, J.K.: *Green Chemistry - Theory and Practical*, OxfordUniversity Press (1998).
6. Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
7. Cann, M.C. &Connely, M.E. *Real-World cases in Green Chemistry*, AmericanChemical Society, Washington (2000).
8. Ryan, M.A. &Tinnesand, M. *Introduction to Green Chemistry*, American ChemicalSociety, Washington (2002).
9. Lancaster, M. *Green Chemistry: An Introductory Text* RSC Publishing, 2nd Edition,2010.

Or

SEC: CHEMOINFORMATICS (30 L) (CHM11027)

Theory: 30 Lectures

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

Hands-on Exercises

Reference Books:

- Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Chemoinformatics.*Springer: The Netherlands.
- Gasteiger, J. & Engel, T. (2003) *Chemoinformatics: A text-book.* Wiley-VCH.
- Gupta, S. P. (2011) *QSAR & Molecular Modeling.* Anamaya Pub.: New Delhi.
- John W. Hill, Terry W. McCreary & Doris K. Kolb, *Chemistry for changing times* 13th Ed.

Industry Academia Interactions/Organization of Seminar CHM14078

Semester V

Physical V **(CHM11072)**

Unit 1: Quantum Mechanics II **(15L)**

Angular momentum **:** Commutation rules, quantization of square of total angular momentum and z-component; Properties of angular momentum operators; Rigid rotator model of rotation of diatomic molecule and Schrödinger equation; Transformation to spherical polar coordinates; Separation of variables; Spherical harmonics; Discussion of solution.

Central force problem: Setting of the Schrödinger equation in Cartesian coordinates, Transformation of coordinate systems, transforming the Schrödinger equation to spherical polar coordinates. Hydrogen atom: separation of variables into radial (r) and angular (Θ and φ) parts, solution of the φ dependent equation and the idea of the magnetic quantum number (m_1), energy expression (no derivation required), idea of degeneracy, the principal (n) and the azimuthal (l) quantum numbers, hydrogen wave functions (up to n=3), the concept of an orbital, real orbitals (suitable linear combinations), radial density distributions, radial and angular nodes, shapes of s, p and d orbitals.

Covalent bonding: Born-Oppenheimer approximation; LCAO-MO treatment of H_2^+; Bonding and antibonding orbitals; Qualitative extension to H_2 ; Comparison of LCAOMO and VB treatments of H_2 and their limitations; Covalent bonding, valence bond and molecular orbital approaches.

Unit 2: Basics of Atomic and Molecular Spectroscopy **(15 L)**

General aspects of spectroscopy, instrumental aspects of specific spectroscopic techniques, applications of molecular symmetry in spectroscopy. Fundamentals and applications of the following methods: Electronic absorption and emission spectroscopy of atoms and molecules, Energy Levels of Atoms and Molecules; Translational, Rotational and Vibrational Energy Levels; Rotational Spectra of Diatomic Molecules; Vibrational Spectra of Diatomic Molecules; IR spectroscopy, Light scattering and Raman spectroscopy.

Unit-3 Photochemistry **(15L)**

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.

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.

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.

Unit 4- Statistical Thermodynamics (15L)

Concept of probability. Microscopic and microstates, thermodynamic probability, entropy and probability, the Boltzmann-Planck entropy formula, the Maxwell-Boltzmann distribution law for the distribution of molecular energies, partition function: molecular and molar, the transitional partition function, thermodynamic quantities from partition function, vibrational partition functions, Einstein's theory of heat capacity of solids, the characteristics temperature, its limitations and Debye's modification.

Nernst heat theorem, approach to zero Kelvin, adiabatic demagnetization, Planck's formulation of third law and the concept of absolute entropies.

References:

1. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 10th Ed., Oxford University
2. Ball, D. W. *Physical Chemistry* Thomson Press, India (2007).
3. Castellan, G. W. *Physical Chemistry* 4th Ed. Narosa (2004).
4. McQuarrie, D. A & Simon, J. D, Physical Chemistry: A molecular approach, Viva student edition
5. Mortimer, R. G. *Physical Chemistry* 3rd Ed. Elsevier: NOIDA, UP (2009).
6. Engel, T. & Reid, P. *Physical Chemistry* 3rd Ed. Pearson (2013).
7. Chatterjee, H. Physical Chemistry, Vol-3, 2nd Edition, Platinum publishers
8. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, (1994), Tata McGraw Hill, New Delhi

Inorganic V (CHM11073)

Unit-1:Bioinorganic Chemistry (20L)

Elements of life: essential major, trace and ultra-trace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^+, K^+, Mg^{2+}, Ca^{2+}, $Fe^{3+/2+}$, $Cu^{2+/1+}$, and Zn^{2+}).Metal ion transport across biological membrane Na^+/K^+-ion pump, ionophores. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins, carbonate bicarbonate buffering system, carbonic anhydrase and carboxypeptidase. Biological nitrogen fixation. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases (examples only).

Unit-2: Organometallic compounds (20 L)

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

Unit-3: Reaction Kinetics and Mechanism (20 L)

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.

References;

1. S.J. Lippard& J.M. Berg,*Principles of Bioinorganic Chemistry*
2. G. N. Mukherjee and A Das, *Bioinorganic Chemistry*
3. Asim K Das, *Bioinorganic Chemistry*
4. B. D. Gupta and A. J . Elias, Organometallic Chemistry
5. R. Sarkar, Vol. 2 *Inorganic Chemistry*
6. F. Basolo and R.C. Pearson, *Mechanisms of Inorganic Chemistry*

Organic V (CHM11074)

Unit 1: Spectroscopy (30L)

NMR Spectra: Nuclear spin, NMR active nuclei, principle of nuclear magnetic resonance,equivalent and non-equivalent carbons and protons, chemical shift δ), shielding / deshielding, upfield and downfield shifts. NMR peak area (integration for PMR), diamagnetic anisotropy, relative peak positions of different kinds of carbons and protons(alkylhalides, olefins, alkynes, aldehyde H), substituted benzenes (toluene, anisole, nitrobenzene, halobenzene, dinitrobenzenes, chloronitrobenzene), first order coupling (splitting of the signals: ordinary ethanol, bromoehane, dibromoehanes), coupling constants.

IR Spectra: Modes of molecular vibrations, application of Hooke's law, characteristic stretchingfrequenciesof O-H, N-H, C-H, C-D, C=C, C=N, C=O functionsand factors effecting stretching frequencies. (H-bonding, mass effect, electronic factors, bond multiplicity, ring size).

UV Spectra: Electronic transition(σ-σ*, n-σ*, π-π* and n-π*), relative positions of λ-maxconsidering conjugative effect, steric effect, solvent effect, red shift (bathochromic shift), blue shift (hypsochromic shift), hyperchromic effect, hypochromic effect (typical examples), Woodward's empirical rule.

Mass spectra: Elementary idea.

Advanced spectroscopy: Spin coupling and coupling constant, interpretation of ^{1}HNMR spectra for some simple systems. Structural elucidation using MS, UV, IR and NMR.

Unit-2-Dynamic stereochemistry (20L)

Selection of substrates: Conformationally rigid and mobile diastereoisomers, single substrate with two or more conformers**;**

Quantitative correlation between conformation and reactivity: Winstein-Elel equation, Curtin-Hamett Principle**;** Conformation, reactivity and mechanism of cyclic and acyclic systems; Formation and reactions of enols and enolates; Reduction of cyclohexanones

Unit 3- Pericyclic Reactions **(10L)**

Electrocyclic reactions: 4e and 6e neutral systems; cycloaddition reactions: [4 + 2] and [2 + 2] reactions, cheletropic addition of carbene; sigmatropic rearrangements: [1,3] and [1,5] H shifts, [3,3] Cope and Claisen rearrangements. FMO analysis and Woodward-Hoffmann selection rules.

Reference Books:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd.(Pearson Education).
3. Kemp, W. *Organic Spectroscopy*
4. Pavia, Lampman and Kriz*Introduction to Spectroscopy*
5. D. Nasipuri*: Stereochemistry of organic compounds: Principles and Applications*
6. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry,* Oxford University Press.
7. Norman &Coxon Principles of Organic Synthesis (CRC Press).

Organic Lab IV (CHM12076)

Further details will be provided during the course

Spectroscopic Analysis of Organic Compounds:

A. Assignment of labelled peaks in the ^{1}H NMR spectrum of the known organic compounds explaining the relative ∂ values and splitting pattern.

B. Assignment of labeled peaks in the IR spectrum of the same compound.

(C-H, O-H, N-H, C=C, C=O, NO2 stretching frequencies)

At least 10-15 compounds from among the list given below are to be chosen:

(i) p-Bromoacetanilide (ii) p-Methyl-α-bromoacetophenone (iii) Vanillin (iv) Cinnamic acid (v) p-Aminobenzoic acid (vi) Salicylamide (vii) o-Hydroxyacetophenone (viii) 4-keto pentanoic acid (ix) Benzylacetate (x) Diethylmaleate (xi) Diethylfumarate (xii) p-Nirtobenzaldehyde (xiv) Mesityl oxide (xv) o-Hydroxybenzaldehyde (xvi) p-Nitroaniline

Refrences:

1. Kemp, W. *Organic Spectroscopy*
2. Pavia, Lampman and Kriz*Introduction to Spectroscopy*
3. D. Nasipuri*: Stereochemistry of organic compounds: Principles and Applications.*

Inorganic Lab IV (CHM12071)

Further details will be provided during the course

Inorganic Preparations:

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

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

iii. Tetraamminecarbonatocobalt (III) ion

iv. Potassium tris(oxalate)ferrate(III)

Chromatography of metal ions

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

i. Ni (II) and Co (II)

Refrences:

1. Subhas C Das, *Advanced Practical Chemistry.*

Discipline specific elective subject for semester V (Choice any two theory and practical papers)

DSE I: Advanced Spectroscopy and its applications (60 L) (CHM11033)

Unit1: Introduction (10L)

Interaction of electromagnetic radiation with matter, transition probabilityand selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy.

Unit2: Rotational and rotation-vibrational spectroscopy (10L)

Di- and polyatomic molecules, normal coordinates and their symmetry (CO_2), skeletal vibration and group frequency, FT-IR instrumentation.

Unit 3. Raman spectroscopy: (5L)

Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines.

Unit 4. Electronic spectroscopy (10L)

Vibronic spectroscopy of diatomic molecules, Franck-Condon factor, dissociation and pre-dissociation, rotational fine structure, solvent effects. Photoelectron spectroscopy (PES): UV and X-ray PES of molecules.

Unit 5. Lasers and laser spectroscopy (10L)

Principles of laser action, laser characteristics, pulsed lasers, laser cavity modes, examples of lasers: He-Ne, Nd-YAG, titanium-sapphire., dye lasers. Lasers in spectroscopy

Unit 6. Magnetic resonance (15L)

A review of spin angular momentum, basic principles and relaxation times, Lintensity of NMR signals, electronic shielding, NMR in liquids: chemical shifts, spin-spin couplings. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals

References:

1. Modern Spectroscopy, J. M. Hollas, 4th edition (2004), John Wiley & Sons, Ltd., Chichester.
2. Introduction to Molecular Spectroscopy, G. M. Barrow, (1962) McGraw-Hill.
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, (1994), Tata McGraw Hill, New Delhi.

DSE I Elective Lab: Advanced Spectroscopy and its applications (CHM12034)

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4)and determine the λ_{max} values. Calculate the energies of the two transitions indifferent units (J molecule-1 kJ mol-1, cm-1, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde,2-propanol, acetic acid) in water. Comment on the effect of structure on the UVspectra of organic compounds.
4. Determine the amount of iron present in a sample using 1, 10-phenathroline.
5. Determine the dissociation constant of an indicator (phenolphthalein).
6. Verification of Beer and Lambert's Law for $KMnO_4$ and $K_2Cr_2O_7$ solution.
7. Determination of the indicator constant of an acid base indicator spectrophotometrically.
8. Study of kinetics of $K_2S_2O_8$+ KI reaction, spectrophotometrically.

References:

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

Or

DSEI: Inorganic Materials of Industrial Importance (60 L) (CHM11035)

Silicate Industries (16L)

Glass: Glassy state and its properties, classification (silicate and non-

silicate glasses).Manufacture and processing of glass. Composition and properties of the following types ofglasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass,fluorosilicate, coloured glass, photosensitive glass.

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

Cements: Classification of cement, ingredients and their role, Manufacture of cement and thesetting process, quick setting cements.

Fertilizers: (8 L)

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

Surface Coatings: (**10 L**)

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

Batteries: (6 L)

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

Alloys: (10 L)

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

Catalysis: (6 L)

General principles and properties of catalysts, homogenous catalysis (catalytic steps andexamples) and heterogenous catalysis (catalytic steps and examples) and their industrialapplications, Deactivation or regeneration of catalysts.Phase transfer catalysts, application of zeolites as catalysts.

Chemical explosives: (4 L)

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

References Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, WileyPublishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, WileyPublishers, New Delhi.
4. J. A. Kent: Riegel's*Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.

DSE I LAB: inorganic materials of industrialimportance lab (CHM12036)

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

References Books:

1. P. C. Jain, M. Jain: *Engineering Chemistry*, DhanpatRai& Sons, Delhi.
2. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, VikasPublications, New Delhi.
3. B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut.

DSE-II: Theoretical Chemistry: (60L) (CHM11041)

Unit-I: FORTRAN programming (15L)

Computer programming in FORTRAN. Syntax for formula translation, Decision making statement, loop, array, subroutine.

Unit-II: Numerical methods revisited (10L)

Differentiation, integration, root determination, differential equation, Matrix manipulation.

Unit-III: Potential energy surface & Energy Minimization (15L)

Coordinate Systems. Potential Energy Surfaces, force field, Electrostatic interactions. van der Waals interactions. Hydrogen bonding.

Minimization and related methods for exploring the energy surface. Derivative and Non-derivative method. Stochastic optimization, Simulated Annealing, Genetic Algorithm. Case study: noble gas cluster, H_2O cluster, polymers.

Unit-4: Molecular Dynamics & Monte Carlo Simulation: (10 L)

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple polymers models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Monte Carlo simulation.

Unit-5: Quantum Chemical Calculation **(10L)**

Born Oppenheimer Approximation, Overview of electronic structure theory. Hatree Fock Method, Self-consistent field (only basics). Basis function. Density functional theory (only basics). Structure determination. Introduction to software for quantum chemical calcution.

Reference Books:

1. Fortran77 and Numerical Methods, C Xavier, New Age International (P) Ltd.
2. Modern Fortran in Practice, Arjen Markus, Cambridge Univrsity Press (2012).
3. Numerical Recipe in Fortran77, The art of scientific computing. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, 2nd Edition, Cambridge Univrsity Press.
4. An introduction to Genetic Algorithm, Melanie Mitchell, The MIT Press
5. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
6. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley andSons, 1997.
7. SatyaPrakash Gupta, QSAR and Molecular Modeling, Springer –AnamayaPublishers, 2008.
8. Quantum Chemistry, I. N. Levine, Prentice Hall.
9. Kirkpatrick K S, Gelatt C D and Vecchi M P 1983 *Science* **220** 671

DSE-III LAB: Theoretical Chemistry **(CHM12042)**

- General Programming
  1. Summation of the terms of series
  2. Swapping and sorting
  3. Numerical Integration, differentiation
  4. Roots of equation
  5. Matrix operations
- Application to real chemical problem
  1. Volume of van der Waal gas (Roots of equation)
  2. Probability distribution function (Numerical Integration)
  3. Potentiometric and pHmetric graph (Numerical differentiation)
- Minimization on Potential energy surface (Steepest descent)
- Introduction to software:
  Molecular Molelling (tinker, CHARM)
  Quantum Chemical calculation (Gaussian)

Reference Books:

1. Fortran77 and Numerical Methods, C Xavier, New Age International (P) Ltd.
2. Modern Fortran in Practice, Arjen Markus, Cambridge Univrsity Press (2012).

3. Numerical Recipe in Fortran77, The art of scientific computing. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, 2nd Edition, Cambridge Univrsity Press.
4. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
5. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley andSons, 1997.

SatyaPrakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

Or

DSE II: Polymer Chemistry (CHM11050)

Unit-1: Introduction and history of polymeric materials: (4 L)
Different schemes of classification of polymers, Polymer nomenclature, Molecular forces andchemical bonding in polymers, Texture of Polymers.

Unit-2: Functionality and its importance: (8 L)
Criteria for synthetic polymer formation, classification of polymerization processes,Relationships between functionality, extent of reaction and degree of polymerization.Bifunctionalsystems, Poly-functional systems.

Unit-3: Kinetics of Polymerization: (4 L)
Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic andanionic) and coordination polymerizations, Mechanism and kinetics of copolymerization,polymerization techniques.

Unit-4: Crystallization and crystallinity: (4 L)
Determination of crystalline melting point and degree of crystallinity, Morphology ofcrystalline polymers, Factors affecting crystalline melting point.

Unit-5: Nature and structure of polymers (**2 L**)

Unit-6: Structure Property relationships: (**8 L**)
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 anditssignificance.Polydispersity index.

Unit-7: Glass transition temperature (T_g) and determination of T_g, (8 L)
Free volume theory, WLFequation, Factors affecting glass transition temperature (T_g).

Unit-8: Polymer Solution (8 L)
Criteria for polymer solubility, Solubility parameter, Thermodynamicsof polymer solutions, entropy, enthalpy, and free energy change of mixing of polymerssolutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

Unit-9: Properties of Polymers (Physical, thermal, Flow & Mechanical Properties). (10 L)

Brief introduction to preparation, structure, properties and application of the followingpolymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and relatedpolymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoropolymers,polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac),polyurethanes, silicone polymers, polydienes,Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylenesulphidepolypyrrole, polythiophene)].

Reference Books:

1. Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
2. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary PolymerChemistry, 3rd ed. Prentice-Hall (2003)
3. Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
4. Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
5. PetrMunk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)

DSE-II LAB: Polymer Chemistry Lab (CHM12051)

Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) /Methyl Acrylate (MA) / Acrylic acid (AA).

a. Purification of monomer

b. Polymerization using benzoyl peroxide (BPO) / 2,2′-azo-bis-isobutylonitrile(AIBN)

2. Preparation of nylon 66/6

1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC)and phenolphthalein

a. Preparation of IPC

b. Purification of IPC

c. Interfacial polymerization

3. Redox polymerization of acrylamide

4. Precipitation polymerization of acrylonitrile

5. Preparation of urea-formaldehyde resin

6. Preparations of novalac resin/resold resin.

7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:

(a) Polyacrylamide-aq.$NaNO_2$ solution

(b) (Poly vinyl proplylidine (PVP) in water

2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol)(PVOH) and the fraction of “head-to-head” monomer linkages in the polymer.

3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG)(OH group).

4. Testing of mechanical properties of polymers.
5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

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

Reference Books:

a) L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley &Sons(2005)
b) Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford UniversityPress (2005)
c) Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

Semester VI

Analytical Chemistry: (CHM11078)

Qualitative and quantitative aspects of analysis: (5 L)
Sampling, evaluation of analytical data, errors, accuracy and precision, methods of theirexpression, normal law of distribution if indeterminate errors, statistical test of data; F, Q andt test, rejection of data, and confidence intervals.

Optical methods of analysis: (20 L)
Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy andselection rules, validity of Beer-Lambert's law.
Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation(choice of source, monochromator, detector, choice of flame and Burner designs. Techniquesof atomization and sample introduction; Method of background correction, sources ofchemical interferences and their method of removal. Techniques for the quantitativeestimation of trace level of metal ions from water samples.

Thermal methods of analysis: (5 L)
Theory of thermogravimetry (TG), basic principle of instrumentation.Techniques for quantitative estimation of Ca and Mg from their mixture.

Electroanalytical methods: (10 L)
Classification of electroanalytical methods, basic principle of pH metric, potentiometric andconductometric titrations. Techniques used for the determination of equivalence points.Techniques used for the determination of pK_a values.

Separation techniques: (20 L)
Solvent extraction: Classification, principle and efficiency of the technique.Mechanism of extraction: extraction by solvation and chelation.Technique of extraction: batch, continuous and counter current extractions.Qualitative and quantitative aspects of solvent extraction: extraction of metal ions fromaqueous solution, extraction of organic species from the aqueous and nonaqueous media.
Chromatography: Classification, principle and efficiency of the technique.Mechanism of separation: adsorption, partition & ion exchange.Development of chromatograms: frontal, elution and displacement methods.Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC,TLC and HPLC.Stereoisomeric separation and analysis: Measurement of optical rotation, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination ofenantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiralchromatographic techniques using chiral columns (GC and HPLC).
Role of computers in instrumental methods of analysis.

Reference Books:

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H.Jeffery and others) 5th Ed. The English Language Book Society of Longman .
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. WardsworthPublishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York,2004.
4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis,Thomson Asia Pvt. Ltd.

Organic VI: (60 L) (CHM11079)

Unit 1- Synthetic Strategy (15L)

Enolate chemistry: Enolates and enamines: formation; alkylation and acylation, reactions withcarbonyls, conjugate addition. Chemistry of acetoacetic ester and malonic ester

Strategy of ring synthesis: thermodynamic factor, synthesis through enolate anion chemistry and carbonyl condensation reactions (including acetoaceticester & malonic ester synthesis),synthesis through rearrangement (including pinacol, Favorski), synthesis of large rings, high dilution technique and acyloin reaction, Stobbe condensation.

Unit-2- Retrosynthetic analysis (30L)

Retrosynthetic analysis: Retrosynthetic analysis- disconnections, synthons, donor and acceptorsynthons,functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-dioxygenated], reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy [alcohol, amine, carbonyl, acid]

Unit-3: Asymmetric synthesis: (15L)

Stereoselective and stereospecific reactions, diastereoselectivity, andenantioselectivity (only definition), diastereoselectivity: addition of nucleophiles to C=O, adjacent to a stereogeniccentre (Felkin-Anh model); addition of electrophiles to C=C (Houk model).

Reference Books:

1. S. Warren: *Organic synthesis: The disconnection approach*
2. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry (1st edition),* Oxford University Press.
3. D. Nasipuri: Stereochemistry of organic compounds: Principles and Applications.

Biological Chemistry (30L) CHM11044

Unit-1: Carbohydrates: (6L)

Monosaccharides: Aldoses upto 6 carbons, structure of D- glucose & D-fructose (configuration & conformation), anomeric effect, mutarotation. Important reactions and conversions including

protection / deprotectionprotocol[osazone formation, bromine – water oxidation, stepping–up (Kiliani method) and stepping–down (Ruff's &Wohl's method)of aldoses]. Disaccharides and poly- saccharide: nature of glycosidic linkages; structure and systematic names of sucrose, lactose, maltose

Unit-2: Aminoacids and peptides: (6L)

Amino acids: Synthesis: (Strecker, Gabriel, acetamidomalonic ester, azlactone); isoelectric point, ninhydrin reaction. Peptides: peptide linkage, synthesis of peptides using N-protection & C-protection, solid phase synthesis; peptide sequence: C-terminal and N-terminal amino acid determination (Edman, Sanger &dansyl chloride).

Problems based on chemical reactions and structure covering the above topics.

Unit-3: Proteins and Nucleic acids: (6L)

Primary, secondary, tertiary and quaternary structure of proteins and protein folding. Nucleic acids: pyrimidine & purine bases (only structure & nomenclature), nucleosides and nucleotides, DNA: Watson-Crick model, complimentary base –pairing in DNA;RNA

Unit-4: Lipids: (6L)

Definition and classification.Fatty acids- properties of saturated and unsaturated fatty acids.Esters of fatty acids-formation and hydrolysis; Essential fatty acids.Triacylglycerols. Reactions and characterization of fats hydrolysis, saponification value, iodine number, rancidity of fats, Reichert- Meissel number. Biological significance of fats.Characterization of fats, Phospholipids, Micelle bilayer, liposomes, Glycolipids, steroids and sterols.

Unit-5: Enzymes (6L)

Cofactors – Definition, examples of a) metal ions b) coenzymes c) prosthetic group, Definition, examples of holoenzymes, Apoenzyme.

Classification of enzymes, IUPAC system, Name & examples of each class Mechanism of enzyme activity—standard free energy change in a reaction-transition state, activation energy both in non-enzymatic and enzymatic reaction, reaction rate, rate constant, rate limiting step, rate equation, binding energy, specificity of enzymes geometric and stereo specificity with example, lock & key hypothesis, induced fit hypothesis.

Reference Books:

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

Allied Knowledge Enhancement Course:

DSE III: Dissertation (CHM15045)

As per choice of research topics by concerned students

Or

DSE III-Environmental Chemistry (CHM11037)

Unit-1: Environment and its segments (20 L)

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.Air Pollution: Major regions of atmosphere.Chemical and photochemical reactions inatmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemicalsmog: its constituents and photochemistry. Environmental effects of ozone, Major sources ofairpollution.Pollution by SO_2, CO_2, CO, NO_x, H_2S and other foul smelling gases.Methods of estimationof CO, NO_x, SO_x and control procedures. Effects of air pollution on living organisms and vegetation.Greenhouse effect and Globalwarming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removalof sulphur from coal.Control of particulates.

Unit-II: Water Pollution: (30 L)

Hydrological cycle, water resources, aquatic ecosystems, Sources andnature of water pollutants, Techniques for measuring water pollution, Impacts of waterpollution on hydrological and ecosystems.Water purification methods. Effluent treatment plants (primary, secondary and tertiarytreatment). Industrial effluents from the following industries and their treatment:electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc.Sludgedisposal.Industrial waste management, incineration of waste. Water treatment and purification(reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water,industrial water and domestic water.

Unit-3: Energy & EnvironmentSources of energy: (10 L)

Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy,Hydrogen, geothermal, Tidal and Hydel, etc.Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management. Biocatalysis: Introduction to biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

References:

1. A. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi
2. Asim. K. Das *Environmental Chemistry with Green Chemistry*

DSE-III LAB: Environmental Chemistry Lab (CHM12038)

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titrationmethod ($AgNO_3$ and potassium chromate).

6. Estimation of total alkalinity of water samples (CO_3^{2-}, HCO_3^-)using double titrationmethod.
7. Measurement of dissolved CO_2.
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid

References:

1. Manahan S.E. (2005) *Environmental Chemistry*, CRC Press

DSE-IV: Chemistry of nanomaterials (60 L) (CHM11046)

Unit-I: Solid state materials (20 L)

Introduction, Crystal structure, Crystalline solids, Crystal systems, Metallic structure-Unit cells, Crystallographic directions and planes, linear and planar densities, close-packed crystal structures, Types of close packing-hcp and ccp, packing efficiency, Ceramics structure- radius ratio. Method of characterization-Powder X-ray diffraction, electron and Neutron diffraction, Thermal analysis, microscopic and spectroscopic techniques as tools for material characterization.Semiconducors - intrinsic and extrinsic, General Strategies for preparation and production of materials: Wet chemical processes, the sol-gel route, precursor synthesis, carbo-thermic and thermo- chemical treatments, hydrothermal, pyrochemical, metallurgical and chemical routes, heat treatment methods, surface.

Unit-II: Nanomaterials: Inorganic and Biomaterials (25L)

Introduction to quantum confinement, Inorganic nanomaterials, General Methods available for the Synthesis of Nanostrutures, reduction-precipitative-reactive-hydrothermal/solvothermal methods-suitability of such methods for scaling-potential Uses; Solution growth techniques of 1D-2D nano structures:- Synthesis of metallic, semiconducting and oxide nanoparticles – homo- and hetero-nucleation growth methods. Nanoclusters and Nanowires; Metal, Metal Oxide, semiconductor nanoparticles, Carbon Nanotubes. Inorganic Materials synthesis by Templating and Self-Assembly; 2-D Nanopatterns and Self-assembled Monolayers on Inorganic Substrates; Mesostructured and Mesoporous Materials; Inorganic-Organic and Inorganic-Polymer Nanocomposite Materials; Protein based nanostructures building blocks and templates, Proteins as transducers and amplifiers of biomolecular recognition events,

Unit-III: Applications in Optoelectronics, Biomedical and Food Industry (20 L)

Inorganic (metal/metal-oxide) nanoparticles in optical devices, light emitting diaplays, nucleic acid and protein based recognition groups, Application in optical detection methods, Nanoparticles in bone substitutes and dentistry, Implants and Prosthesis, Reconstructive Intervention and Surgery, Photodynamic Therapy, Nanobiosensors in Diagnosis, Inorganic metal oxide/lanthanides as MRI agents, Drug delivery, Therapeutic applications, Artificial life, Hybrid materials, Future of Bionanotechnology. Fertilizer and pesticides. Smart delivery

system, Insecticides using nanotechnology, Potential of nano-fertilizers, Nanotechnology in Food industry.

Reference Books:

1. C. N. R. Rao, A. Muller, A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Volume 1, Wiley-VCH, Verlag GmbH, Germany (2004).
3. Guozhong Cao, *Nanostructures & Nanomaterials Synthesis, Properties G;Z: Applications*, World Scientific Publishing Private, Ltd., Singapore (2004).
4. Carl C. Koch, *Nanostructured Materials: Processing, Properties and Potential Applications*, Noyes Publications, William Andrew Publishing Norwich, New York, U.S.A (2002).
C. M. Niemeyer, C. A. Mirkin-*Nanobiotechnology: Concepts, Applications and Perspectives*‖, Wiley – VCH, (2004).
5. T. Pradeep, ―*Nano: The Essentials*‖, McGraw – Hill education, (2007).

DSE-IV LAB: Chemistry of Nanomaterials Lab (CHM12047)

1. Synthesis of micelles and inverse micelles.
2. Synthesis of Silica sol and gel nanoparticles.
3. Preparation of thiolated silver nanoparticles.
4. Synthesis of Gold Nanoparticles by chemical and biogenic methods.
5. Zinc sulphide quantum dot preparation.
6. Synthesis of Iron Oxide Nanoparticle.
7. Thin film preparation by spin coating technique.
8. Synthesis of Nickel metal nanoparticle by urea decomposition method.
9. Synthesis of Zinc Oxide and cadmium oxide nanoparticles.
10. Preparation of nanoparticles by using Ball milling.

References:

1. T. Pradeep, ―*Nano: The Essentials*‖, McGraw – Hill education, (2007).
2. Challa, S.S.R. Kumar, Josef Hormes, Carola Leuschaer, *Nanofabrication Towards Biomedical Applications, Techniques, Tools, Applications and Impact*‖, Wiley – VCH, (2005).
Bharat Bhushan,*Springer Handbook of Nanotechnology*, Barnes & Noble (2004).
3. Neelina H. Malsch (Ed.),*Biomedical Nanotechnology,* CRC Press (2005)

Or

DSE-IV: Green Chemistry and Chemistry of Natural Products (CHM11048)

Unit 1: Introduction to Green Chemistry (4 L)

What is Green Chemistry? Need for Green Chemistry.Goals of Green Chemistry.Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit 2: Principles of Green Chemistry and Designing a Chemical synthesis (24 L)

Twelve principles of Green Chemistry with their explanations and examples; Designing aGreen Synthesis using these principles; Prevention of Waste/ byproducts; maximumincorporation of the materials used in the process into the final products (Atom Economy);prevention/ minimization of hazardous/ toxic products; designing safer chemicals – differentbasic approaches to do so; selection of appropriate auxiliary substances (solvents, separationagents), green solvents, solventless processes, immobilized solvents and ionic liquids; energyrequirements for reactions - use of microwaves, ultrasonic energy; selection of startingmaterials; avoidance of unnecessary derivatization – careful use of blocking/protectinggroups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents;designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardoussubstances in chemical processes.

Unit 3: Examples of Green Synthesis/ Reactions (24 L)

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methylmethacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide,acetaldehyde, disodium iminodiacetate (alternative to Strecker synthesis), citral, ibuprofen,paracetamol, furfural.

2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzylchloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Oxidation (oftoluene, alcohols). Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification ofesters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles fromaldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.

3. Ultrasound assisted reactions: Esterification, saponification, substitution reactions,Alkylations, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

4. Selective methylation of active methylene group using dimethylcarbonate: Solid-statepolymerization of amorphous polymers using diphenylcarbonate; Use of "Clayan", anonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role ofTellurium in organic syntheses; Biocatalysis in organic syntheses.

Unit 4: Future Trends in Green Chemistry (8 L)

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial greenchemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistryin sustainable development.

Reference Books:

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

2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistryexperiment*. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American ChemicalSociety, Washington DC (2002).

DSE-IV LAB: Green Chemistry and Chemistry of Natural Products Lab (CHM12049)

1. Safer starting materials

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

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

2. Using renewable resources

Preparation of biodiesel from vegetable oil.

3. Avoiding waste

Principle of atom economy.

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

Preparation of propene by two methods can be studied

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

(II) 1-propanol $\xrightarrow{H_2SO_4/\Delta}$ pr propene + water

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

4. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

Alternative Green solvents

5. Diels Alder reaction in water

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

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

7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis (C_2S_3) of N-organophthalimide using phthalicanhydride and 3-aminobenzoic acid.

Alternative sources of energy

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

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

Reference books:

Sharma, R.K.; Sidhwani, I.T. &Chaudhari, M.K. I.K. *Green Chemistry Experiment:A monograph International Publishing House Pvt Ltd. New Delhi*. Bangalore CISBN978-93-81141-55-7 (2013).