SEMESTER-II M 2 CHE 02-CT 06 Organic Chemistry

Time: 3 Hrs.

M.M. 80 marks (External)
20 marks (Internal)
Credits = 4

UNIT-I

Stereochemistry

Elements of symmetry, Chirality, Molecules with more than one chiral center, DL, RS and EZ nomenclature, methods of resolution, Optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereo specific and stereo selective synthesis, optical activity in the absence of chiral carbon (biphenyl, allenes and spiranes), chirality due to helical shape. Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity.

UNIT-II

Asymmetric Synthesis

Inroduction to asymmetric synthesis, Cram's and Prelog's rules. Use of chiral auxiliaries, chiral catalyst (L-Proline based reaction), asymmetric hydrogenation, asymmetric epoxidation (Sharpless epoxidation), and asymmetric dihydroxylation, Enzyme catalyzed asymmetric reactions (Reduction and oxidations).

UNIT-III

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements - Pinacol-Pinacolone rearrangement, Wagner- Meerwin rearrangement, Demjanov rearrangement, Benzil - Benzilic acid rearrangement, Favorskii rearrangement, Wolff rearrangement, Neber rearrangement, Beckmann rearrangement, Hofmann rearrangement, Curtius rearrangement, Schmidt

rearrangement, Lossen rearrangement, Bayer-Villiger rearrangement and Stevens rearrangement.

UNIT-IV

Reagents in organic synthesis: Use of the following reagents in organic synthesis and functional group transformation, Gilman's reagent, lithium dimethyl cuprate LDA, dichlorohexylcarbodiimide, trimethyl silyl iodide, tributyltin hydride, DDQ, Baker yeast, Petersons synthesis, Merrifield resins, 1,3-dithiane, selenium oxide, osmium tetroxide, use of N-heterocyclic carbene in organic synthesis.

UNIT-V

Pericyclic reactions

Introduction, classification of pericyclic reactions, molecular orbital symmetry, frontier orbitals of ethylene, 1,3 –butadiene, 1,3,5-hexatriene and allyl system. Woodward Hoffmann Correlation diagram, F.M.O. and PMO approach to cycloaddition and electrocyclic reactions. Electrocyclic reactions- Conrotatory and disrotatory motions, 4n and 4n+2. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloaddition and cheleotropic reactions.

Sigmatropic rearrangement-suprafacial and antrafacial shifts of H, Sigmatropic shifts involving carbon moieties, Claisen, Cope and aza-Cope rearrangement. Fluxional tautomerism. Ene reaction.

Books Recommended:

- Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum
- 3. Modern Organic Reactions, H.O. House, Benjamin
- 4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
- 5. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.

- 6. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 7. Stereochemistry of Organic Compounds, P.S Kalsi, New age International.
- 8. Organic Reaction and Their Mechanisms, P.S. Kalsi, New Age International.
- 9. Organic Reaction Mechanism, V.K. Ahluwalia and R.K. Parshar, New Age International.
- 10. Stereochemistry of Organic Compounds, E.L. Eliel.

SEMESTER-II M 2 CHE 03-CT 07 Physical Chemistry

Time: 3 Hrs.

M.M. 80 marks (External)
20 marks (Internal)
Credits = 4

UNIT-I

Classical thermodynamics: Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies, partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significance, determinations of these quantities.

Non-ideal systems: Excess function for non-ideal solutions, activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolyte solutions, determination of activity and activity coefficients, ionic strength.

UNIT-II

Statistical thermodynamics - Concept of distribution, thermodynamic probability and most probable distribution, ensemble averaging, postulates of ensemble averaging, canonical, grand canonical, and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers)Partition function, translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, applications of partition functions. Chemical equilibrium and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, Bose-Einstein statistics, distribution law.

UNIT-III

Non-equilibrium thermodynamics —Meaning of Irreversible(Non-equilibrium) thermodynamics, Thermodynamic criteria for non-equilibrium states, phenomenological lawslinear laws, Gibbs equation, Onsager reciprocal relations, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc.) Prigogines principal of maximum entropy production, transformations of the generalized fluxes and forces. Applications of non-equilibrium thermodynamics.

UNIT-IV

Surface chemistry - Surface tension, Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces. Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, solubilization, microemulsion, reverse micelles.

UNIT-V

Electrochemistry: Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Debye-Huckel-Jerum mode, derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination, structure of electrified interfaces, Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models, over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, semiconductor interfaces, theory of double layer at semiconductor, electrolyte - solution interfaces, structure of soluble layer interfaces, effect of light at semiconductor solution interface.

Book Recommended:

- 1. Modem Electrochemistry Vol. I and Vol.II, J.O.M. Bockris and A.K.N. Reddy, Plenum
- 2. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed. Wiley
- 3. McQuarrie, D. A. Statistical Mechanics Viva Books Pvt. Ltd.: New Delhi (2003).
- 4. Nash, L. K. Elements of Statistical Thermodynamics 2nd Ed., Addison Wesley (1974).
- 5. Physical Chemistry, P.W Atkins, ELBS
- 6. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum

SEMESTER-II M 2 CHE 04-CT 08 Environmental and Green Chemistry

Time: 3 Hrs.

M.M. 80 marks (External)
20 marks (Internal)
Credits = 4

UNIT I

Principle and concepts of Green Chemistry:-Introduction, definition, principles, atom economy, atom economic and atom uneconomic reaction, reducing toxicity.

Waste- Production, Problems and Preventions: Introduction, problem caused by waste, source of waste, cost of waste, waste minimization techniques, on-site waste treatment, design for degradation, polymer recycling. Introduction to catalysis, biocatalyst and phase transfer catalysis.

UNIT-II

Green Solvents: Organic solvents, solvent-free systems, controlling of solvent-free reactions, supercritical fluids (H₂O and CO₂), fluorous biphase solvents.

Green Reagents: Introduction, methods of designing safer chemicals, avoidance of toxic functional groups, examples of greener reagents including replacement of phosgene, methylations using dimethyl carbonates and other polymer supported reagents, solid state polymerization, alternative nitrile synthesis.

UNIT-III

Green Synthesis: Design for energy efficiency, classification and applications of Green Synthesis including Microwave Assisted Synthesis green synthesis of polycarbonates, paracetamol, ibuprofen, citral, urethane, adipic acid, styrene, α , β -unsaturated nitroalkenes.

UNIT-IV

Environmental chemistry: Atmosphere –chemical and photochemical reactions in the atmosphere, oxygen and ozone Chemistry, greenhouse gases and effect, hydrosphere-physical chemistry of sea water, eutrophication, sewage treatment, lithosphere and chemistry involved, smoke formation acid rains. A brief idea of toxicological effects of arsenic, lead, cadmium

mercury, ozone PAN, cyanide and pesticides. Oxide of nitrogen, sulphur and carbon, carcinogens.

UNIT-V

Analysis of pollution: Sampling and monitoring of air and water, determination of total dissolved solids, conductivity, acidity, alkalinity, harmness, chloride, sulphate, fluoride phosphate and different forms of nitrogen phenols, pesticides, surfactants DO, BOD, COD and microorganism. Catalysts of aquatic chemical reactions water pollution laws and standards.

Books Recommended:

- 1. Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of Chemicals, Cambridge,
- 2. Green Chemistry: Frontiers in Benign Chemical Synthesis and Processes, Edited by Paul T. Anastas & Tracy C. Williamson, Oxford University Press.
- 3. Green Chemical Syntheses and Processes: Edited by Paul T. Anastas, Lauren G. Heine & Tracy C. Williamson, ACS Symposium Series.
- 4. Green Chemistry: Environment Friendly Alternatives, Edited by Rashmi Sanghi, M. M. Srivastava, Narosa Publishing House, New Delhi.
- 5. Green Chemistry: Microwave Synthesis, K. R. Desai, Himalaya Publishing House.
- 6. Green Chemistry: A Teaching Resource, Dorothy Warren, Royal Society of Chemicals, 2001.
- 7. Green Chemistry: Williams, Charlotte.
- 8. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
- 9. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
- 10. Environmental Chemistry, A. K. De, Wiley Eastern.
- 11. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern

- 12. Standard Method of Chemical Analysis, F.J. Welcher Vol. Ill, Van Nostrand Reinhold Co.
- 13. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
- 14. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
- 15. Environmental Chemistry, C. Baird, W. H. Freeman.

SEMESTER-II M 2 CHE 05-CP 03 (Core Practical-3) Credits 4; Time 8h Inorganic Chemistry

M.M. 80 marks (External) 20 marks (Internal)

I. Water Analysis - (minimum -4)

- 1. Determination of hardness of water
- 2. Determination of BOD in water sample
- 3. Determination of COD in water sample
- 4. Determination of DO in water sample
- 5. Determination of available Chlorine in water sample
- 6. Determination of Fluoride in water

II. Analysis of purity of chemicals (-3)

- 1. Determination of available oxygen in hydrogen peroxide
- 2. Determination of phosphoric acid in phosphoric acid
- 3. Determination of available chlorine in bleaching powder

III. Volumetric estimation (-4)

- 1. Determination of Al, Ba, Ca, Cu, Fe, Cr, Ni and Co using complexometric titration
- 2. Determination of Fe²⁺, nitrite by cerimetry
- 3. Determination of Iodide, Sn²⁺ by Potassium iodate

IV. Chromatography (-3)

Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/nonaqueous media:

- (i) Pb²⁺ and Ag⁺ (aqueous & non-aqueous media)
- (ii) Co^{2+} and Cu^{2+} (non-aqueous medium)
- (iii) Cl⁻ and I⁻ (aqueous-acetone medium)
- (iv) Br and I (aqueous-acetone medium)

V. Analysis of Electronic Spectra (-1)

Analysis of Electronic Spectra of transition metal complexes at least for one system [dn (Oh) or (Td)] and calculation of Crystal, Field parameters, interelectronic repulsion parameter and bonding parameter.

SEMESTER-II M 2 CHE 06-CP 04 (Core practical-4) Physical Chemistry + Organic Chemistry

Credits 4; Time 8h

M.M. 80 marks (External) 20 marks (Internal)

Physical Chemistry

1. Distribution law

- I. Complex formation between copper sulphate and ammonia.
- II. Equilibrium constant of the reaction between iodine and potassium iodide.
- III. Study the distribution of benzoic acid in benzene and water to show the benzoic acid dimerise in benzene,

2. Conductometry – (minimum -4)

- I. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
- II.Find out the equivalent conductance of strong electrolytes (NaCl, KCl, KNO₃, HCl etc.) at different dilutions and verify Debye-Huckel-Onsager equation.
- III. Determination of velocity constant and order of the reaction for saponification of ethyl acetate by sodium hydroxide conductometrically.
- IV. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.
- V. Study the estimation of potassium sulphate solution by conductometric titration. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with Sodium hydroxide.

Organic Chemistry

1. Quantitative Analysis (minimum -2)

- I. Determination of equivalent weight of an acid by silver salt method
- II. Estimation of phenol/aniline using Bromate-Bromide solution or by acetylation method

- III. Estimation of glucose by titration using Fehling's solution/ Benedict solution
- **IV.** Estimation of carbonyl group by using 2, 4-dinitrophenylhydrazine.
- 2. Analysis of oils and fats (minimum -2)
- I. Determination of saponification value of oil.
- II. Determination of iodine value of oil.
- III. Determination of acid value of oil.
- 3. Chromatography of amino acids and carbohydrates:-
- I. Separation of components by TLC
- II. Separation of components by adsorption paper chromatography