II SEMESTER

TITRIMETRIC AND APPLIED ANALYSIS			
Course Code	MSC201	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To familiarize statistical methods to validate analytical methods.
- To learn sampling techniques and conventional volumetric methods.
- To study basic theories of air pollution, and water pollution methods.
- To learn principles and instrumentations of several analytical techniques to determine pollutants.
- To learn the several pollutants and their determinations.

Module-1

Obtaining and preparing samples for analysis: Importance of sampling, designing a sample plan-random, judgement, systematic-judgement, stratified and convenience sampling. Type of sample to collect - grab and composite samples. Insitu sampling. Size of sample and number of samples. Implementing the sampling plan - solutions, gases and solids. Bringing solid samples into solution - digestion and decomposing.

Titrimetric analysis: An overview of titrimetry. Principles of titrimetric analysis. Titration curves. Titrations based on acid-base reactions - titration curves for strong acid and strong base, weak acid and strong base and weak base and strong acid titrations. Selecting and evaluating the end point. Finding the end point by visual indicators, monitoring *p*H and temperature.

Quantitative applications – selecting and standardizing a titrant, inorganic analysis - alkalinity, acidity and free CO_2 in water and waste waters, nitrogen, sulphur ammonium salts, nitrates and nitrites, carbonates and bicarbonates. Organic analysis - functional groups like carboxylic acid, sulphonic acid, amine, ester, hydroxyl, carbonyl. Air pollutants like SO_2. Quantitative calculations. Characterization applications - equivalent weights and equilibrium constants.

Module-2

Acid-base titrations in non-aqueous media: Role of solvent in acid-base titrations, solvent systems, differentiating ability of a solvent, some selected solvents, titrants and standards, titration curves, effect of water, determining the equivalence point, typical applications - determination of carboxylic acids, phenols and amines.

Precipitation titrations: Titration curves, feasibility of precipitation titrations, factors affecting shape - titrant and analyte concentration, completeness of the reaction, titrants and standards, indicators for precipitation titrations involving silver nitrate, Volhard, Mohr and Fajan's methods, typical applications.

Module-3

Complexometric titrations: Complex formation reactions, stability of complexes, stepwise formation constants, chelating agents, EDTA - acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves - completeness of reaction, indicators for EDTA titrations - theory of common indicators, titration methods employing EDTA - direct, back and displacement titrations, indirect determinations, titration of mixtures.

Redox titrations: Balancing redox equations, calculation of the equilibrium constant of redox reactions, calculating titration curves, detection of end point, visual indicators and potentiometric end point detection. Quantitative applications-adjusting the analyte's oxidation state, selecting and standardizing a titrant. Inorganic analysis- chlorine residuals, dissolved oxygen in water, water in non-aqueous solvents.

Organic analysis-chemical oxygen demand (COD) in natural and waste waters, titrations of mercaptans and ascorbic acid with I_3^- and titration of organic compounds using periodate.

Module-4

Air pollution, analysis and control: Historical overview - global implications of air pollution, sources of pollutants, classification of pollutants. Sources and effects of particulates, carbon monoxide, sulphur oxides, nitrogen oxides, hydrocarbons and photochemical oxidants on human health, vegetation and materials. Standards for air pollutants.

Air quality monitoring: Sampling methods and devices for particulates and gaseous pollutants. SO_2: ambient air measurements and stack gas measurements - Turbidimetric, colorimetric, conductometric and coulometric methods, NOX: Griess-ilosvay and Jacobs-Hockheiser colorimetric methods, chemiluminiscent technique, CO: NDIR, amperometric, FID and catalytic oxidation methods. Hydrocarbons: total and individual hydrocarbons by gas chromatography. Oxidants and ozone: colorimetric, coulometric, titrimetric and chemiluminescence methods.

Air Pollution control: Atmospheric cleaning processes, approaches to contaminant control-detection and control at source.

Control devices for particulates: Gravitational settlers, centrifugal collectors, wet collectors, electrostatic precipitation and fabric filtration.

Control devices for gaseous pollutants: adsorption, absorption, condensation and combustion processes. Automative emission control-catalytic converters.

Module-5

Water pollution and analysis: Water resources, origin of wastewater, types of water pollutants; their sources and effects, chemical analysis for water pollution control - objectives of analysis, parameters of analysis, sample collection and preservation. Environmental and public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, chlorine demand, sulphate, fluoride, phosphates and different forms of nitrogen in natural and waste/polluted waters, heavy metal pollution - public health significance of Pb, Cd, Cr, Hg, As, Cu, Zn and Mn, general survey of the instrumental techniques for the analysis of heavy metals in aquatic systems, organic loadings - significance and measurement of DO, BOD, COD, TOD, and TOC, phenols, pesticides, surfactants and tannin and lignin as water pollutants and their determination.

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001, John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prenticeHall, Inc. New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders CollegePublishing, California, 1990.
7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
9. Standard Methods of Chemical Analysis, A.J. Weleher (Part B), Robert E. KriegorPublishing Co. USA,

1975.
10. Environmental Chemistry, S.E. Manahan Willard grant press, London, 1983.
11. Environmental Chemical Analysis, Iain L Marr and Malcolm S. Cresser, Blackie and Son Ltd., London, 1983.
12. Chemistry for Environmental Engineering, Chair N. Sawyer and Perry L.M Canty, Mcgraw Hill Book, Co., New York, 1975.
13. The Air Pollution Hand Book, Richard Mabey, Penguin, 1978.
14. The Pollution Hand Book, Richard Mabey, Ponguin 1978.
15. Soil Chemical Analysis, M.L. Jackson, Prentice Hall of India Pvt, Ltd., New Delhi, 1973.
16. Experiments in Environmental Chemistry, P.D. Vowler and D.W. Counel, Pergamon press, Oxford 1980.
17. Manual Soil Laboratory Testing, vol I, K.H. Head, Pentech Press, London 1980.
18. A Text Book of Environmental Chemistry and Pollution Control, S.S. Dara, S. Chand and co. Ltd. New Delhi 2004.
19. Air pollution Vol II edition by A.C. Stern, Academic Press New York, 1968.
20. Instrumental Methods for Automatic Air Monitoring Systems in Air Pollution Control, Part-III edition by W. Stranss, John-Wiley and Sons, New York, 1978.
21. Analysis of Air pollutants, P.O. Warner, John Wiley and Sons, New York, 1976.
22. The Chemical Analysis Air pollutants, Interscience, New York, 1960.
23. The Analysis of Air Pollutants, W. Liethe, Ann Arbor Science Pub. Inc. Michigan 1970.
24. Environmental Chemistry, A. K. De.

Course Outcomes: After the completion of this course, the students gain the knowledge of;

CO1	Sampling, purification, characterizations and data analysis using instrumental techniques.
CO2	Foundation of chemical principles for understanding the behavior of chemical constituents in samples
CO3	Basic Principle of Instrumentation and analytical applications
CO4	Basic theories of air pollution, and water pollution methods
CO5	Principles and instrumentations of several analytical techniques to determine pollutants.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	**X**						
CO2	**X**						
CO3	**X**	**X**	**X**				
CO4	**X**	**X**	**X**			**X**	**X**
CO5	**X**	**X**	**X**			**X**	**X**

COORDINATION AND ORGANOMETALLIC CHEMISTRY			
Course Code	MSC202	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To understand the preparation, properties, electronic configuration and structural elucidation of coordination compounds.
- To learn the reaction mechanism, stereochemistry and photochemistry of coordination compounds.
- To understand the fundamental concepts of organometallic chemistry and general principles of homogeneous and heterogeneous catalysis.
- To learn the concepts of metal clusters, silicates and silicones.

Module-1

Preparation of coordination compounds: Introduction, Preparative methods- simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions. Geometries of metal complexes of higher coordination numbers (2-12).

Stability of coordination compounds: Introduction, trends in stepwise stability constants, factors influencing the stability of metal complexes with reference to the nature of metal ion and ligands, the Irving-William series, chelate effect.

Determination of stability constants: Theoretical aspects of determination of stability constants of metal complexes by spectrophotometric and polarographic methods.

Crystal field theory: Salient features of CFT, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, Jahn-Teller distortions, measurement of 10 Dq and factors affecting it. Evidences for metal-ligand covalency.

Molecular Orbital Theory: MOT to octahedral, tetrahedral and square planar complexes without and with pi-bonding.

Module-2

Electronic spectra: Introduction, selection rules and intensities, electronic spectra of octahedral and tetrahedral complexes, Term symbols for d^n ions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra. Ligand-field transition. Charge transfer and energy applications. Optical rotatory dispersion and Circular dichroism. Magnetic circular dichroism.

Magnetic properties: Introduction, magnetic susceptibility and its measurements, spin and orbital contributions to the magnetic moment, the effects of temperature on μeff, spin-cross over, ferromagnetism, anti-ferromagnetism and ferrimagnetism.

Applications of infrared spectroscopy of coordination compounds: Metal complexes of ammine, nitro, nitrito, hydroxo, carbonato, sulphato, cyano, cyanato and thiocyanato complexes.

Module-3

Reactions and Mechanisms: Introduction. Substitution reactions- Inert and labile compounds, mechanisms of substitution. Kinetic consequences of Reaction pathways- Dissociation, interchange and association.Experimental evidence in octahedral substitution- Dissociation, associative mechanisms, the conjugate base mechanism, the kinetic chelate effect.

Stereochemistry of reactions- Substitution in *trans* and its complexes, isomerization of chelate rings. Substitution reactions of square-planar complexes-kinetics and stereochemistry of square-planar substitutions, evidence for associative reactions, explanations of the *trans* effect.

Electron-transfer processes: Inner-sphere mechanism and outer-sphere mechanism, conditions for high and

low oxidation numbers.

Photochemistry of coordination compounds: Photochemistry of chromium(III) ammine compounds, Light-induced excited state spin trapping in iron(II) compounds and MLCT photochemistry in pentammineruthenium(II) compounds.

Module-4

Fundamental concepts of Organometallics Chemistry: Introduction, Classification of organometallic compounds by bond type, nomenclature, the effective atomic number rule, complexes that disobey the EAN rule, common reactions used in complex formation.

Organometallics of transition metals: Preparation, bonding and structures of nickel, cobalt, iron and manganese carbonyls. Preparation and structures of metal nitrosyls.

Ferrocene: Preparation, structure and bonding**. Metal-carbene and metal-carbyne complexes**.

Complexes containing alkene, alkyne, arene and allyl ligands: Preparation, structure and bonding.

Module-5

General principles of Catalysis: Language of catalysis. Homogeneous and heterogeneous catalysts.

Homogeneous catalysis - Industrial Applications: Alkene hydrogenation and hydroformylation, The Wacker's process, Monsanto acetic acid process and L-DOPA synthesis, alkene oligomerizations, water-gas shift reactions. The Reppe reaction.

Heterogeneous catalysis –The nature of heterogeneous catalysts. Alkene polymerization: Ziegler-Natta catalysis, Fischer-Tropsch carbon chain growth. New directions in heterogeneous catalysis.

Zeolites as catalysts for organic transformation: Uses of ZSM – 5.

Alkene metathesis, hydroboration, arylation or vinylation of olefins (Heck reaction).

Biological and Medicinal Applications: Organomercury, organoboron, organosilicon and organoarsenic compounds.

References

1. Physical Inorganic Chemistry- A Coordination Chemistry Approach- S.F.A. Kettle, Spektrum, Oxford, (1996).
2. Inorganic Chemistry-4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
3. Inorganic Chemistry-5th edition. G.L. Miessler, P. J. Fischer and D.A. Tarr, Pearson (2014).
4. Inorganic Chemistry-6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
5. Inorganic Chemistry- 3rd edition, James E. Huheey, Harper and Row Publishers, (1983).
6. Basic Inorganic Chemistry- 3rd edition, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons, (2002).
7. Infrared and Raman Spectra of Coordination Compounds, Part-B- 6th edition, K. Nakamoto, John Wiley and Sons (2009).
8. Organometallic Chemistry, 2nd edition, R.C. Mehrothra and A. Singh, New Age International Publications (2006).
9. The Organometallic Chemistry of the Transition Metals, 4th edition, Robert H. Crabtree, Wiley Interscience, (2005).
10. Organometallics - A Concise Introduction, 2nd edition, ChistophElschenbroich and Albert Salzer VCH, (1992).
11. Inorganic Chemistry, 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson

Education Ltd., (2005).
12. Inorganic Chemistry- 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education,(2004).
13. Basic Organometallic Chemistry - B.D. Gupta and A.J. Elias, Universities Press (2010).
14. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
15. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
16. Organometallic Chemistry and Catalysis, Didier Astruc, Springer (2007).

Course Outcomes:

CO1	Gain the knowledge of preparative methods of coordination compounds and geometries of different coordination numbers.
CO2	Understand the CFT and MOT bonding theories to metal complexes.
CO3	Electronic spectra, magnetic properties and infrared spectroscopy of coordination compounds. In addition, understand the reaction mechanism and photochemistry of coordination compounds.
CO4	Fundamental concepts of organometallic chemistry and synthesis, structure and bonding in different organometallics and their applications.
CO5	Homogeneous and heterogeneous catalysts and their applications in the synthesis of organic compounds in industries and Chemistry of main group elements, metal clusters, silicates and silicones and their applications in day to day life

Mapping of COs and POs

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**						
CO2	**X**						
CO3	**X**						
CO4	**X**	**X**	**X**			**X**	**X**
CO5	**X**	**X**	**X**			**X**	**X**

SYNTHETIC ORGANIC AND BIOORGANIC CHEMISTRY			
Course Code	MSC203	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	60	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To understand the reactions of organic compounds involving various reagents.
- To learn the synthesis and retro-synthesis of different organic compounds.
- To learn the synthesis and biological importance of carbohydrates, proteins and nucleic acid.

Module-1

Oxidation: Oxidation with chromium and manganese reagents (CrO_3, $K_2Cr_2O_7$, PCC, PDC, Sarret reagent, MnO_2, $KMnO_4$, ozone, peroxides and peracids, periodic acid, OsO_4, SeO_2, NBS, Oppenauer oxidation, Sharpless epoxidation.

Reduction: Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Ra-C, Ni, Ru, Rh), solvents and reduction of functional groups, catalytic hydrogen transfer reactions. Wilkinson catalyst, $LiAlH_4$, $NaBH_4$, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination), diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, Wolff-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride, Bakers yeast, Organoboron compounds: Introduction and preparations. Hydroboration and its applications. Reactions of organoboranes: isomerization reactions, oxidation, protonolysis, carbonylation, cyanidation. Reactions with aldehydes or ketones (*E* and *Z*-alkenes).

Module-2

Reagents and reactions in organic synthesis: Use of following reagents in organic synthesis and functional group transformations: Lithium diisopropylamide (LDA), Gilmann reagent, dicyclohexyl carbodimide (DCC), dichlorodicyanoquinone (DDQ), Silane reagents-trialkylsilyl halides, trimethylsilyl cyanide, trimethyl silane, phase transfer catalyst, crown ethers, cyclodextrins, Ziegler- Natta catalyst, diazomethane, Woodward and Prevost hydroxylation, Stark enamine reaction, phosphorous ylides - Wittig and related reactions, sulphur ylides – reactions with aldehydes and ketones, 1,3-dithiane anions - Umpolung reaction, Peterson reaction. Palladium reagents: Suzuki coupling, Heck reaction, Negishi reaction. Green Chemistry: Definition and principles, planning green synthesis in the laboratory, green preparations- aqueous reactions, solid state (solvent free) reactions, photochemical reactions, enzymatic transformations and reactions in ionic liquids.

Module-3

Molecular rearrangements: Introduction Carbon to carbon migration: Pinacol-pinacolone, Wagner-Meerwein, Benzidine, benzylic acid, Favorskii, Fries rearrangement, dienophile rearrangement. Carbon to nitrogen migration: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements. Miscellaneous rearrangements: Wittig, Smiles, Bayer-Villeger rearrangement and Barton reaction.

Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Synthons and synthetic equivalents. Retrosynthesis and synthesis of benzofurans, *p*-methoxy acetophenone, saccharine, α-bisabolene, nuciferal, tetralone, ibuprofen, functional group transformations in organic synthesis; nitro to keto, nitro to aniline, acid to alcohol etc..

Module-4

Carbohydrates: Carbohydrates: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosaccharides, anomeric effect, Hudson's rules, epimerization and mutarotation. Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose,

maltose and lactose. Polysaccharides: General methods of structure elucidation. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar- agar. Photosynthesis and biosynthesis of carbohydrates.

Module-5

Amino Acids: General structure, physiological properties, protection of functional groups.

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt, Synthesis of oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic). Proteins: Structure determination: *C* and *N* terminal residue determination, primary, secondary, tertiary and quartenary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach and phosphoramide methods. Solid phase synthesis of oligonucleotides. Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins.

References

1. 1 Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-I & II by I. L. Finar.
3. Advance Organic Chemistry, IV edition, Jerry March.
4. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechard J. Sundberg.
5. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
6. Organic named reactions and molecular rearrangements, Gudeep Raj.
7. Modern synthetic reactions, II edition, H. O. House.
8. Organic synthesis, Jagadamba Singh and L. D. S. Yadav.
9. Green Chemistry, K. R. Desai.
10. Principles of Organic synthesis, R. O. C. Norman and J. M. Coxon.
11. Organic synthesis II edition, V. K. Aluwalia and Renu Agarwal.
12. Organic synthesis, Robert E. Ireland.
13. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
14. Organic chemistry by Clayden, Greeves, Warren and Wothers.

Course Outcomes:

CO1	Students are familiar about chemistry of oxidants, reductants and their applications in the organic synthesis.
CO2	Understand the various catalysts in organic synthesis by known naming reactions.
CO3	Retro-synthesis and molecular rearrangement.
CO4	Synthesis, industrial and biological importance of carbohydrates.
CO5	General synthesis of amino acids, peptides, nucleic acids and their biological significance.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	**X**	**X**					
CO2	**X**	**X**	**X**				
CO3	**X**	**X**	**X**			**X**	**X**

CO4	**X**	**X**	**X**			**X**	**X**
CO5	**X**	**X**	**X**			**X**	**X**

PRINCIPLES OF PHYSICAL AND SURFACE CHEMISTRY			
Course Code	MSC204	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	3	Exam Hours	3

Course Learning Objectives:

- To understand the basics of polymers, their kinetics and applications.
- To understand the general principles of catalysis and enzyme kinetics.
- To understand the physico-chemical principles of biological fluids.
- To learn the pharmaco kinetics, pharmaco dynamics, toxico kinetics of biological systems.
- To study fundamentals and theoretical background on the concepts of surface chemistry

Module-1

Polymers: Fundamentals of polymers - monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers, Polymerization - condensation, addition, free radical, ionic, co-ordination polymerization and ring opening polymerization. Molecular weight and size, polydispersion. Average molecular weight concepts – number, weight and viscosity average molecular weight. Determination of molecular weights - viscosity method, osmotic pressure method, sedimentation and light scattering methods. Kinetics of Polymerization - Condensation, addition, free radical, ionic, co-ordination polymerization. Phase transitions in polymers and thermal characterization: Glass transition, crystallinity and melting- correlation with the polymer structure. Polymers in solution: Criteria of polymer solubility, thermodynamics of polymer solutions. Colloids: Types and classification, Micelles: Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, micellar catalysis

Module-2

Homogeneous Catalysis: Electronic and structural effects on acidity and basicity. Hard and soft acids and bases. Acidity functions: Hammet acidity function, Zucker-Hammet hypothesis, Bonnett hypothesis. Industrial catalysis: Catalyst carrier, promoter, inhibitor and catalyst poison.

Enzyme kinetics: Effect of substrate concentration (Michaelis - Menton equation), Effect of pH, effect of catalysts and inhibitors (substrate, zeolite, Cr3+, Fe2+ ZnO, U.V light), effect of temperature. A brief kinetic and mechanistic applications of glucose oxidase in the oxidation of glucose.

Linear Free Energy Relationship: Hammett equation, Taft equation, Okemoto Brown equation and its application to oxidation of amino acids and aromatic amines. Swain- Scott and Edward equation. Winstein - Grunwald relationship. Isokinetic relationship and significance of isokinetic temperature, Exner criterion.

Kinetic Isotope Effect: Theory of kinetic isotope effect - normal and inverse isotope effect, primary isotope effect, secondary isotope effect, solvent isotope effect.

Module-3

Biophysical Chemistry: Electrophoresis - Principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electro-osmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. Micelles and its involvement during digestion and absorption of dietary lipids. Diffusion of solutes across bio-membranes and its application in the mechanism of respiratory exchange. “Salting In” and “Salting Out” of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Effect of temperature and pH on the viscosity of bio-molecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension.

Biological significance of surface tension - stability of Alveoli in lungs, interfacial tension in living cells (Danielli and Davson model). Application of sedimentation velocity and sedimentation equilibrium method for molecular weight determination of proteins.

Module-4

Pharmacokinetics: Introduction, biopharmaceutics, pharmacokinetics, clinical pharmacokinetics, pharmacodynamics, toxicokinetics and clinical toxicology. Measurement of drug concentration in blood, plasma or serum. Plasma level-time curve, significance of measuring plasma drug concentrations.

One compartment open model: Intravenous route of administration of drug, elimination rate constant, apparent volume of distribution and significance. Calculation of elimination rate constant from urinary excretion data, clinical application.

Two compartment model: Plasma level-time curve, relationship between tissue and plasma drug concentrations, Apparent volumes of distribution. Drug clearance, clinical example. Plasma level-time curve for a three compartment open model. Drug absorption: Factors affecting the rate of drug absorption - nature of the cell membrane, Route of drug administration - Oral drug absorption, Intravenous infusion and intravenous solutions, Effect of food on gastrointestinal drug absorption rate.

Module-5

Surface Chemistry: Review of adsorption curves, adsorption-desorption, adsorption forces, heat of adsorption and types. Measurement of heat of adsorption (Calorimetric and Clausius Clapeyron methods). Measurement of adsorption isotherms, (Volumetric and Gravimetric methods). Determination of entropy of adsorption, Electrostatic adsorption. Adsorption indicators and their applications. Volcanic curves, Applications of adsorption.

Adsorption Theories: Polanyi's potential theory and Polarization theory, Hysteresis of adsorption. *Surface Structure*: Surface mobility, Surface heterogeneity, Surface area and its determination by point-B method. Harkins-Jura method. Radioactive tracer method and Benton and White method. Importance of surface area. Examination of surfaces by Interferometer method. Scanning electron microscopy (SEM), Low energy electron diffraction method (LEED method). Field Emission spectroscopy. Auger electron spectroscopy (AES), STM, and TEM.

References

1. Polymer Science. V. R. Gowrikar, N.V. Vishwanathan and J. Sreedhar, Wiley Eastern, New Delhi (1990).
2. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta, Tata – McGraw Hill New Delhi (1978).
3. Polymer Characterization, D. Campbell and J.R. White, Chapman and Hall, New York.
4. Fundamental Principles of Polymer Materials, R.L. Rosen, John Wiley and Sons, New York.
5. Introduction to Physical Organic Chemistry, R.D. Gilliom, Madison – Wesley, USA (1970).
6. Physical Organic Chemistry- Reaction Rate and Equilibrium Mechanism – L.P. Hammett, McGraw HillBook, Co., (1970).
7. Biophysical Chemistry- Principle and Technique – A. Upadhyay, K. Upadhyay and N. Nath, Himalaya Publishing House, Bombay, (1998).
8. Essentials of Physical Chemistry and Pharmacy – H. J. Arnikar, S. S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).
9. Applied Biopharmacokinetics and Pharmacokinetics - Leon Shargel, Andrew YuPrentice-Hall International, Inc (4^{th} edition).
10. Essentials of Physical Chemistry and Pharmacy – H.J. Arnikar, S.S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).
11. Physical Chemistry of Surfaces - A. W. Adamson, Interscience Publishers Inc., New York (1967).

12. Surface Chemistry: Theory and Applications - J. J Bikertman, Academic Press, New York (1972).
13. Physical Chemistry - R. J. Silbey. R. A. Alberty and M G Bawendi, Wiley (2009).
14. Physics at Surfaces – A. Zangwill, Cambridge University Press (1988).
15. Surface Crystallography - L. J Clarke, Wiley, Interscience (1985).

Course Outcomes: After the completion of this course, the students have

CO1	Fundamentals of polymers and their applications in controlling the quality and waste management of polymer product.
CO2	Knowledge about catalysis and enzyme kinetics
CO3	Gain the knowledge on theory and principles of biophysical chemistry and pharmacokinetics.
CO4	This course helps to understanding the bio-availability and different pharmacokinetic parameters of drugs in the living system.
CO5	Fundamentals and theoretical background on the concepts of surface chemistry

Mapping of COs and POs

	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**
CO1	**X**						
CO2	**X**						
CO3	**X**	**X**					
CO4	**X**		**X**			**X**	
CO5	**X**	**X**	**X**			**X**	

ANALYTICAL CHEMISTRY PRACTICALS			
Course Code	MSCL205	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	84	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives:

- To understand basic concepts by carrying out analytical experiments.
- The experimental results are subjected to validation of analytical parameters.

PART-A

1. Determination of total acidity of vinegar and wines by acid-base titration.
2. Determination of purity of a commercial boric acid sample, and Na_2CO_3 content of washing soda.
3. Analysis of chromate-dichromate mixture by acid-base titration.
4. Determination of replaceable hydrogen and relative molecular mass of a weak organic acid by titration with NaOH.
5. Determination of ephedrine and aspirin in their tablet preparations by residual acid-base titrimetry.
6. Determination of purity of aniline and assay of chlorpromazine tablets by non-aqueous acid- base titration.
7. Periodate determination of ethylene glycol and glycerol (Malprade reaction).
8. Determination of carbonate and bicarbonate in a mixture by *p*H-metric titration and comparison with visual acid-base titration.
9. Determination of purity of a commercial sample of mercuric oxide by acid-base titration.
10. Determination of benzoic acid in food products by titration with methanolic KOH in chloroform medium using thymol blue as indicator.
11. Determination of the *p*H of hair shampoos and *p*H determination of an unknown soda ash.
12. Analysis of water/waste water for acidity by visual, *p*H metric and conductometric titrations.
13. Analysis of water/waste water for alkalinity by visual, *p*H metric and conductometric titrations.
14. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and *p*H-titrimetry.
15. Determination of ammonia in house-hold cleaners by visual and conductometric titration.
16. Potentiometric determination of the equivalent weight and Ka for a pure unknown weak acid.
17. Spectrophotometric determination of creatinine and phosphorus in urine.
18. Flame emission spectrometric determination of sodium and potassium in river/lake water.
19. Spectrophotometric determination of *p*Ka of an acid-base indicator.

PART-B

1. Determination of percentage of chloride in a sample by precipitation titration-Mohr, Volhard and Fajan's methods.
2. Determination of silver in an alloy and Na_2CO_3 in soda ash by Volhard method.
3. Mercurimetric determination of blood or urinary chloride.
4. Determination of total hardness, calcium and magnesium hardness and carbonate and bicarbonate hardness of water by complexation titration using EDTA.
5. Determination of calcium in calcium gluconate/calcium carbonate tablets/injections and of calcium in milk powder by EDTA titration.

6. Analysis of commercial hypochlorite and peroxide solution by iodometric titration.
7. Determination of copper in an ore/an alloy by iodometry and tin in stibnite by iodimetry.
8. Determination of ascorbic acid in vitamin C tablets by titrations with KBrO3 and of vitamin C in citrus fruit juice by iodimetric titration.
9. Determination of iron in razor blade by visual and potentiometric titration using sodium metavanadate.
10. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.
11. Determination of nickel in steel by synergic extraction and boron in river water/sewage using ferroin.
12. Determination of total cation concentration of tap water by ion-exchange chromatography.
13. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.
14. Cation exchange chromatographic separation of cadmium and zinc and their estimation by EDTA titration.
15. Gas chromatographic determination of ethanol in beverages.
16. Determination of aspirin, phenacetin and caffeine in a mixture by HPLC.
17. Solvent extraction of zinc and its spectrophotometric determination.
18. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.
19. Separation and determination of chloride and bromide on an anion exchanger.
20. Thin layer chromatographic separation of amino acids.

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
8. Practical Clinical Biochemistry by Harold Varley and Arnold.Heinmann, 4th edition.

Course Outcomes:

CO1	Develop the skill to carry out acid-base titrimetric analysis, potentiometric and conductometric methods.
CO2	Understand the chemistry of different chemical reactions involved in the determination of pharmaceutical, industrial and vegetable samples.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	**X**	**X**					
CO2	**X**	**X**	**X**	**X**		**X**	**X**

ORGANIC CHEMISTRY PRACTICALS			
Course Code	MSCL206	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	1:6:0	SEE Marks	50
Total Hours of Pedagogy	84	Total Marks	100
Credits	4	Exam Hours	3

Course Learning Objectives:

- To understand synthetic methods by carrying out different experiments.
- To develop the skill for the separation and qualitative analysis of binary mixtures of organic compounds.

PART-A

1. Preparation *p*-nitroaniline from acetanilide**.**
2. Preparation of *n*-butyl bromide from *n*-butyl alcohol.
3. Preparation of chalcone.
4. Preparation of osazone
5. Preparation of phenoxyacetic acid
6. Preparation of 7-hydroxy-4-methyl coumarin
7. Preparation of hippuric acid from glycine
8. Preparation of aniline from nitrobenzene
9. Preparation of s-benzylisothiouronium chloride
10. Preparation of benzoic acid from benzaldehyde

PART-B

Qualitative analysis: Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives.

References

1. Vogel' text book of practical organic chemistry, V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatehell.
2. Elementary practical organic chemistry, Part-I: Small scale preparations, Part-II: Qualitative organic analysis, By Arthur I, Vogel.
3. Hand book of organic analysis, H. T. Clarke and Norman Collie.
4. Experiments in Organic Chemistry, Louis F. Fieser.
5. Laboratory manual of Organic Chemistry by B. B. Dey and M. V. Sitaraman.
6. Practical Organic Chemistry by Mann F. G. and Saunders.

Course Outcomes:

CO1	Students are involved in the multi-step synthesis of different organic compounds.
CO2	Understand the qualitative analysis of binary mixture of organic compounds through separation, identification of functional groups and preparation of some solid derivatives.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	**X**	**X**	**X**			**X**	**X**
CO2	**X**	**X**	**X**			**X**	**X**