

COURSE STRUCTURE

Sem.	Course No.	Courses	L T P	Credit Hr.
III	Theory			
	ACC13120	Inorganic Chemistry-I	3 – 0 – 0	06
	ACC13121	Organic Chemistry-I	3 – 0 – 0	06
	APC 93102	Optics	4 – 0 – 0	08
	AMC13101	Methods of Applied Mathematics-I	4 – 1 – 0	09
	ESE13101	Environmental Chemistry	4 – 1 – 0	09
	Practical			
	ACC13220	Inorganic Chemistry Lab – I	0 – 0 – 3	03
	APC93201	Optics Lab	0 – 0 – 3	03
	ESE13201	Environmental Chemistry Lab	0 – 0 – 3	03
		Total	18 – 2 – 9	47

Sem.	Course No.	Courses	L T P	Credit Hr.
IV	Theory			
	ACC14122	Physical Chemistry – I	3 – 0 – 0	06
	ACC14123	Inorganic Chemistry – II	3 – 0 – 0	06
	ACC14124	Organic Chemistry – II	3 – 0 – 0	06
	APC94102	Electricity & Magnetism	3 – 0 – 0	06
	AMC14101	Numerical and Statistical methods	4 – 0 – 0	08
	Practical			
	ACC14222	Physical Chemistry Lab – I	0 – 0 – 3	03
	ACC14223	Organic Chemistry Lab – I	0 – 0 – 3	03
	APC94201	Electricity & Magnetism Lab	0 – 0 – 3	03
	AMC14201	Numerical and Statistical Methods Practical	0 – 0 – 3	03
	Co-curricular activity			
	SWC34701	Co-Curricular Activity	0 – 0 – 0	03
		Total	16 – 0 – 12	47

Sem.	Course No.	Courses	L T P	Credit Hr.
V	Theory			
	Core Courses			
	ACC15125	Physical Chemistry – II	3 – 1 – 0	07
	ACC15126	Inorganic Chemistry – III	3 – 1 – 0	07
	ACC15127	Organic Chemistry – III	3 – 1 – 0	07
	CSR15101	Data Structure	3 - 0 - 0	06
	ACC15141	Introduction to Biochemistry	3 – 0 – 0	06
	Practical			
	ACC152 25	Physical Chemistry Lab – II	0 – 0 – 3	03
	ACC152 26	Inorganic Chemistry Lab – II	0 – 0 – 3	03
	ACC152 27	Organic Chemistry Lab – II	0 – 0 – 3	03
	Term paper			
	ACC15601	Term paper		02
	ACC15402	Seminar		02
Total			15 – 3 – 9	46

Sem.	Course No.	Courses	L T P	Credit Hr.	
VI	Theory				
	ACC16128	Physical Chemistry – III	3 – 1 – 0	07	
	ACC16129	Inorganic Chemistry – IV	3 – 1 – 0	07	
	ACC16130	Organic Chemistry – IV	3 – 1 – 0	07	
	CSR16102	Computer Networks	3 - 0 - 0	06	
	HSC36107	Communication Skills	3 – 1 – 0	07	
	Practical				
	ACC 16228	Physical Chemistry Lab- III	0 – 0 – 3	03	
	ACC16229	Inorganic Chemistry Lab-III	0 – 0 – 3	03	
	ACC16230	Organic Chemistry Lab – III	0 – 0 – 3	03	
	Co-curricular activity				
	SWC-34701	Co-Curricular Activity	0 – 0 – 0	03	
	Total			15 – 4 – 9	46

Sem.	Course No.	Courses	L T P	Credit Hr.
VII	Theory			
	ACC31131	Physical Chemistry – IV	3 – 1 – 0	07
	ACC31132	Organic Chemistry – V	3 – 1 – 0	07
	ACC31133	Inorganic Chemistry – V	3 – 1 – 0	07
	ACC31134	Analytical Chemistry – I	3 – 1 – 0	07
	ACC31147	Chemistry of Materials	3 – 0 – 0	06
	Practical			
	ACC31231	Chemistry Practical – I	0 – 0 – 3	03
	ACC31232	Chemistry Practical – II	0 – 0 – 3	03
	ACC32233	Chemistry Practical – III	0 – 0 – 3	03
		Total	15 – 4 – 9	43

Sem.	Course No.	Courses	L T P	Credit Hr.	
VIII	Theory				
	ACC32135	Physical Chemistry – V	3 – 1 – 0	07	
	ACC32136	Organic Chemistry – VI	3 – 1 – 0	07	
	ACC32137	Inorganic Chemistry – VI	3 – 1 – 0	07	
	ACC32138	Introduction to Group Theory	3 – 0 – 0	06	
	CSR16101	Data Base Management System	3 – 1 – 0	07	
	Practical				
	ACC32239	Computer Application in Chemistry Lab	0 – 0 – 3	03	
	ACC32234	Chemistry Practical – IV	0 – 0 – 3	03	
	ACC32235	Chemistry Practical- V	0 – 0 – 3	03	
	Seminar				
	ACC32402	Seminar	0 – 0 – 0	03	
			Total	15 – 4 – 9	46
	Summer Training				
ACC-329 01	Summer Training Project (3 weeks)				

Sem.	Course No.	Courses	L T P	Credit Hr.
IX	Theory			
	Core Courses			
	ACC-33140	Solid State Chemistry and Photochemistry	3 – 0 – 0	06
	ACC-33142	Analytical Chemistry – II (Instrumental Methods)	3 – 0 – 0	06
	HSC-21103	Scientific writing	2 – 2 – 0	06
	Elective Courses (One from each group I, II)			
	Group I			
	ACE-33143	Surface Chemistry and Catalysis	3 – 0 – 0	06
	ACE-33144	Organic Synthesis	3 – 0 – 0	06
	ACE-33145	Advanced Electrochemistry	3 – 0 – 0	06
	Group II			
	ACE-33151	Bioinorganic Chemistry	3 – 0 – 0	06
	ACE-33153	Bioorganic and Medicinal Chemistry	3 – 0 – 0	06
	Practical etc			
	ACC-332 36	Chemistry Practical – VI	0 – 0 – 3	03
	ACC-332 37	Chemistry Practical – VII	0 – 0 – 3	03
	ACC-332 38	Chemistry Practical – VIII	0 – 0 – 3	03
	Seminar/Summer Training Project Report			
	ACC-334 01	Seminar	0 – 0 – 0	03
ACC-338 02	Summer Training Project Report	0 – 0 – 0	06	
		Total	14 – 2 – 9	48

Sem.	Course No.	Courses	L T P	Credit Hr.
X	Theory			
	Core Course			
	ACC-34146	Applications of spectroscopy in Organic and in Inorganic Chemistry	3 – 1 – 0	07
	Elective Courses (One each from Grp. I, II)			
	Group I			
	ACE-34148	Organometallic Chemistry	3 – 1 – 0	07
	ACE-34150	Electron, Nuclear and Radiation Spectroscopy	3 – 1 – 0	07
	ACE-34154	Waste Utilization	3 – 1 – 0	07
	Group II			
	ACE-34155	Science of corrosion and corrosion control	3 – 1 – 0	07
	ACE-34152	Electrochemical energy system	3 – 1 – 0	07
	ACE-34149	Chemistry of macromolecules	3 – 1 – 0	07
	Project/Seminar/Dissertation/Viva-voce			
	ACC-34301	Project work	0 – 0 – 15	15
	ACC-34402	Seminar	0 – 0 – 0	03
	ACC-34803	Dissertation and viva-voce	0 – 0 – 0	06
			Total	9 – 3 – 15

III SEMESTER*Theory*ACC13120 *Inorganic Chemistry – I (3 0 0)***Periodic Properties**

Atomic and ionic radii, ionization energy, electron affinity and electronegativity – definition, methods of determination or evaluation, trends in periodic table and applications in predicting and explaining the chemical behaviour.

Chemical Bonding

Covalent Bond – Valence bond theory and its limitations, directional characteristics of covalent bond, various types of hybridization and shapes of simple inorganic molecules and ions. Valence shell electron pair repulsion (VSEPR) theory to NH_3 , H_3O^+ , SF_4 , ClF_3 , ICl_2 and H_2O . MO theory, homonuclear diatomic molecules, multicenter bonding in electron deficient molecules, bond strength and bond energy, percentage ionic character from dipole moment and electronegativity difference.

Ionic Solids – Ionic structures, radius ratio effect and coordination number, limitation of radius ratio rule, lattice defects, semiconductors, lattice energy and Born-Haber cycle, solvation energy and solubility of ionic solids, polarizing power and polarisability of ions, Fajan's rule. Metallic bond-free electron, valence bond and band theories.

Weak Interactions – Hydrogen bonding, van der Waals forces.

s-Block Elements

Comparative study, diagonal relationships, salient features of hydrides, solvation and complexation tendencies including their function in biosystems, an introduction to alkyls and aryls.

p-Block Elements

Comparative study (including diagonal relationship) of groups 13-17 elements, compounds like hydrides and halides of groups 13-16, hydrides of boron-diborane and higher boranes, borazine, borohydrides, fullerenes, carbides, fluorocarbons, silicates (structural principle, basic properties of halogens, interhalogens and polyhalides).

Chemistry of Noble Gases

Chemical properties of the noble gases, chemistry of xenon, structure and bonding xenon compounds.

ACC13121 **Organic Chemistry – I (3 0 0)**

Structure and Bonding: Hybridization, bond lengths and bond angles, bond energy, localized and delocalized chemical bond, van der Waals interactions, resonance, hyperconjugation, aromaticity, inductive and field effects, hydrogen bonding.

Mechanism of Organic Reactions: Different types of organic reactions. Energy considerations. Reactive intermediates – carbocations, carbanions, free radicals and carbenes

Stereochemistry of Organic Compounds

Concept of isomerism. Types of isomerism.

Alkanes, Alkenes, Alkynes and Cycloalkanes: Nomenclature, preparation, properties and chemical reactions.

Arenes and Aromaticity: Nomenclature of benzene derivatives. The aryl group. Aromatic nucleus and side chain. Structure of benzene: molecular formula and Kekule structure. Stability and carbon-carbon bond lengths of benzene, resonance structure, MO picture.

Aromaticity: the Huckel rule, aromatic ions.

Aromatic electrophilic substitution – general pattern of the mechanism, role of σ - and π - complexes. Mechanism of nitration, halogenation, sulphonation, mercuration and Friedel-Crafts reaction. Energy profile diagrams. Activating and deactivating substituents, orientation and ortho/para ratio. Side chain reactions of benzene derivatives. Birch reduction.

Methods of formation and chemical reactions of alkylbenzenes, alkynylbenzenes and biphenyl.

Alkyl and Aryl Halides: *Nomenclature and classes of alkyl halides, methods of formation, chemical reactions. Mechanisms of nucleophilic substitution reactions of alkyl halides, S_N2 and S_N1 reactions, substitution at the allylic and vinylic positions of alkenes.*

Methods of formation of aryl halides, nuclear and side chain reactions. The addition-elimination and the elimination-addition mechanisms of nucleophilic aromatic substitution reactions.

APC93102 Optics (4 0 0)

Geometrical Optics:

Fermat's Principle: Principle of extremum path, aplanatic points of a sphere and other applications.

General theory of image formation: Cardinal points of an optical system, general relationship, thick lens and lens combinations. Lagrange's equation of magnification, telescopic combination, telephoto lenses and eyepieces.

Aberration in images: Chromatic aberrations, achromatic combination of lenses in contact and separated lenses, Monochromatic aberrations and their reductions; aspherical mirrors and Schmidt corrector plates, aplanatic points, oil immersion objectives, meniscus lens.

Optical instruments: Entrance and exit pupils, need for a multiple lens eyepiece, common types of eyepieces.

Physical Optics:

Interference of light: The principle of superpositions, two-slit interference, coherence requirement for the sources, optical path retardations, lateral shift of fringes, Rayleigh refractometer and other applications. Localised fringes; thin films, applications for precision measurements for displacements.

Haidinger fringes: Fringes of equal inclination. Michelson interferometer, its application for precision determination of wavelength, wavelength difference and the width of spectral lines. Twyman-Green interferometer and its uses. Intensity distribution in multiple beam interference, Tolansky fringes, Fabry-Perot interferometer and etalon.

Fresnel diffraction: Fresnel half-period zone plates, straight edge, rectilinear propagation

Fraunhofer diffraction: Diffraction at a slit, half-period zones, phasor diagram and integral calculus methods, the intensity distribution, diffraction at a circular aperture and a circular disc, resolution of images, Rayleigh criterion, resolving power of telescope and microscope systems, outline of phase contract microscopy.

Diffraction gratings: Diffraction at N parallel slits, intensity distribution, plane diffraction grating, reflection grating and blazed gratings. Concave grating and different mountings. Resolving power of a grating and comparison with resolving powers of prism and of a Fabry-Perot etalon

Double refraction and optical rotation: Refraction in uniaxial crystals, its electromagnetic theory. Phase retardation plates, double image prism. Rotation of plane of polarization, origin of optical rotation in liquids and in crystals, Applications.

AMC13101 Methods of Applied Mathematics-I (4 1 0)

Section A: Analysis of complex Variables: Limit, Continuity and differentiability of function of Complex variables. Analytic Functions, Cauchy-Riemann's and Cauchy's integral theory, Morera's theorem, Cauchy's integral formula, Expansions of functions of complex variables in Taylor's series and Laurent's series, Singularities and poles. Residue theorem, contour integration, conformal mappings and its applications, Bilinear Transformations.

Section B: Special Functions: Solution in series of ordinary differential equations, Solution of Bessel and Legendre Equations, recurrence relations and generating function for $J_n(X)$, Orthogonal Property and integral representations of $J_n(X)$. Legendre Polynomials, Rodrigue's formula, Orthogonality Properties and generating functions for $P_n(X)$. Elliptic integrals and Error Function and their properties.

Section C: Laplace Transform and PDE: Laplace transform of simple functions, first and second sifting theorems, t -multiplications and t -divisions theorems; Laplace transforms of derivatives, integral and periodic functions. Inverse Laplace transform and convolution property. Use of Laplace transform in evaluating complicated and improper integrals and solution of ordinary differential equations related to engineering problems.

Partial Differential Equations: Classification of partial differential equations, Solution of one dimensional wave equations, one dimensional unsteady heat flow equation and two dimensional steady heat flow equation in Cartesian and polar coordinates by variable separable method with reference to Fourier trigonometric series and by Laplace transform technique.

ESE13101 Environmental Chemistry (4 1-0)

Environmental Chemistry of Water:

The principles and application of aqueous chemistry to the environmental systems. Unique properties of water, Water Quality Parameters: physico-chemical, biological, bacteriological; Xenobiotics; Water Quality Criteria and Standards; Water quality monitoring and management aspects, Chemical methods involved in treating water and wastewater, Removal of dissolved organics and inorganics, Heavy metal pollution and its abatement. Natural water pollution: Eutrophication, Detergents and phosphates, Removal of nitrogen and phosphates, Water disinfection. Significant of water quality parameters.

Atmospheric Chemistry:

Structure and properties of atmosphere, Classification and chemistry of major air pollutants and their control. Types and sources of air pollution-natural, Combustion and other combustion sources. Thermodynamics and kinetics of air pollutants. Atmospheric photochemistry, Chemical and photochemical reactions in atmosphere. Atmospheric pollution due to automobile emissions and its control, Smog, PAH, VOCs, Acid rain, Depletion of stratospheric ozone. Control devices for gaseous pollutants with especial emphasis on adsorption, absorption, mass transfer, condensation, and combustion.

Soil Chemistry:

The nature and importance of soil; Soil in the natural and man-made environment, Soil properties; Acid-Base and Ion-exchange reactions in soils. Macro and Micronutrients; Fertilisers and other soil amendments. Waste and pollutants in soil, Heavy metals and radio-nuclides in soil. Colloidal chemistry of inorganic constituents, clays, OM and soil humus; Absorption in soils - forces and isotherms; Soil as cation and anion exchanger; Degradation of natural substances; Remediation of metal contaminated soil.

Environmental Chemistry of Hazardous Substances:

Classification and characteristics of hazardous substances and wastes, Effects and fate of Hazardous wastes. Reduction, treatment and disposal of hazardous wastes with special reference to chemical treatment. Photolytic reactions.

Practical

ACC13220 Inorganic Chemistry Lab- I (0 0 3)

Semimicro Analysis- cation analysis, separation and identification of ions from Group I, II, III, IV, V and VI. Anion analysis.

APC 93201 Optics Lab (0 0 3)

Determination of Wavelength of sodium light by Newton's ring.
Determination of Wavelength of sodium light by Fresnel's bi-prism.
Determination of Refractive index of prism by Spectrometer.
Determination of frequency of tuning fork by Melde's experiment.
Determination of velocity of sound in the material of the given rod with a Kundt's tube.

ESE 13201 Environmental Chemistry Lab (0 0 3)

Calibration and Standardisation of pH meter, Conductivity meter, Nephelometer and other water quality monitoring instrument; Determination of pH, Acidity-Alkalinity, Total suspended solids (TSS), Total dissolved solids (TDS), Total hardness and Ca & Mg hardness, Chloride, Sulphate, Nitrate, Oil and grease, DO, BOD, COD, Chlorine demand, Break-point chlorination and Free residual chlorine.
Soil sampling, Description of the soil horizon, Determination of soil pH, Conductivity and Salinity; Organic carbon, Nitrogen and Phosphorus; Sodium and Potassium; CEC, Available sulphur.
Sampling and analysis of inorganic and organic particulates, SO_x , NO_x , NH_3 etc.
Demonstration of UV-VIS Spectrophotometer, Flame photometer, AAS, GC, TOC etc.

IV SEMESTER

Theory

ACC14122 Physical Chemistry – I (3 0 0)

Gaseous State

Postulates of kinetic theory of gases, deviation from ideal behavior, van der Waals equation of state.

Critical Phenomena : PV isotherms of real gases, continuity of states, the isotherms of van der Waals equation, relationship between critical constants and van der Waals constants, the law of corresponding states, reduced equation of state.

Molecular velocities : Root mean square, average and most probable velocities. Qualitative discussion of the Maxwell's distribution of molecular velocities, collision number, mean free path and collision diameter. Liquification of gases (based on Joule-Thomson effect).

Liquid State

Intermolecular forces, structure of liquids (qualitative description). Structural differences between solids, liquids and gases. Liquid crystals: Difference between liquid crystal, solid and liquid.

Solid State

Definition of space lattice, unit cell. Laws of crystallography – Law of constancy of interfacial angles, Law of rationality of indices, Law of symmetry. Symmetry elements in crystals. X-ray diffraction by crystals. Derivation of Bragg equation. Determination of crystal structure of NaCl, KCl and CsCl (Laue's method and powder method).

Colloidal State

Definition and classification of colloids. Solids in liquids (sols): properties – kinetic, optical and electrical; stability of colloids, protective action, Hardy-Schulze law, gold number. Liquids in liquids (emulsions): types of emulsions, preparation. Emulsifier. Liquids in solids (gels): classification, preparation and properties, inhibition, general application of colloids.

Chemical Kinetics

Chemical kinetics and its scope, rate of a reaction, factors influencing the rate of a reaction. Concentration dependence of rates, mathematical characteristics of simple chemical reactions – zero order, first order, second order, pseudo order, half life and mean life. Determination of the order of reaction – differential method, method of integration, method of half life period and isolation method.

Effect of temperature on rate of reaction, Arrhenius equation, concept of activation energy, Simple collision theory based on hard sphere model, transition state theory (equilibrium hypothesis). Expression for the rate constant based on equilibrium constant and thermodynamic aspects.

ACC14123 Inorganic Chemistry – II (3 0 0)

Chemistry of Elements of First Transition Series

Characteristic properties of d-block elements.

Properties of the elements of the first transition series, their binary compounds and complexes illustrating relative stability of their oxidation states, coordination number and geometry.

Chemistry of Elements of Second and Third Transition Series

General characteristics, comparative treatment with their 3d-analogues in respect of ionic radii, oxidation states, magnetic behaviour spectral properties and stereochemistry.

Oxidation and Reduction

Use of redox potential data – analysis of redox cycle, redox stability in water – Front, Latimer and Pourbaix diagrams. Principles involved in the extraction of the elements.

Coordination Compounds

Werner's coordination theory and its experimental verification, effective atomic number concept, chelates, nomenclature of coordination compounds, isomerism in coordination compounds, valence bond theory of transition metal complexes.

Chemistry of Lanthanide Elements

Electronic structure, oxidation states and ionic radii and lanthanide contraction, complex formation, occurrence and isolation, lanthanide compounds.

Acids and Bases

Arrhenius, Bronsted-Lowry, the Lux-Flood, solvent system and Lewis concept of acids and bases.

Non-aqueous Solvents

Reactions in non-aqueous solvents with reference to liquid NH₃ and liquid SO₂.

ACC14124 Organic Chemistry – II (3 0 0)***Alcohols***

Classification and nomenclature. Methods of preparation and properties.

Phenols

Nomenclature, structure and bonding. Preparation of phenols, physical properties and acidic character. Comparative acidic strengths of alcohols and phenols, resonance stabilization of phenoxide ion. Reactions of phenols .

Ethers and Epoxides

Nomenclature of ethers and methods of their formation, physical properties. Chemical reactions – cleavage and autoxidation, Zeisel's method.

Synthesis of epoxides. Acid and base-catalyzed ring opening of epoxides, orientation of epoxide ring opening, reactions of Grignard and organolithium reagents with epoxides.

Aldehydes , Ketones and carboxylic acids: Nomenclature, synthesis and reactions.

Carboxylic Acid Derivatives

Structure and nomenclature of acid chlorides, esters, amides (urea) and acid anhydrides. Physical properties, interconversion of acid derivatives by nucleophilic acyl substitution.

Preparation of carboxylic acid derivatives, chemical reactions. Mechanisms of esterification and hydrolysis (acidic and basic).

Organic Compounds of Nitrogen

Preparation of nitroalkanes and nitroarenes. Chemical reactions of nitroalkanes. Mechanisms of nucleophilic substitution in nitroarenes and their reductions in acidic, neutral and alkaline media. Picric acid.

Structure and nomenclature of amines, physical properties. Chemical properties and reactivity.

APC94102 Electricity & Magnetism (3 0 0)

Electric field: Coulomb's law; unit of charge (SI and other systems of units), Conservation and quantisation of charge; field due to different charge distributions, monopole, dipole, quadrupoles, line charge, sheet charge. Torque on a dipole in uniform field and non-uniform fields, flux of an electric field. Gauss's law; applications to deduce E fields, force per unit area on the surface of a charged conductor.

Potential: Line integral of electric field and electrical potential; field as the gradient of potential. Potential energy of a system of charges; pair of charges, line charge, sheet charge, spherical shell of charge, charged hollow disc. Field equations for E in vacuum. Energy associated with E field. Differential form of Gauss' divergence law, Poisson's equation, Laplace's equation, boundary conditions, and Uniqueness theorems.

Electric field around conductors: Induced charges; field and potential inside a conductor, field near the surface of a conductor, method of images.

Electric fields in matter: Atomic and molecular dipoles; induced dipoles, polarisability tensor, electronic and molecular contributions. Electrical field caused by polarized matter, E and D fields, permittivity, dielectric constant. Capacitor field with a dielectric, field equations in presence of dielectric. The field of a polarized sphere, dielectric sphere in a uniform field. Energy in dielectric systems; polarisability and susceptibility, frequency dependence of polarisability, Clausius-Mossotti equation.

Magnetic effect of current: A critical review.

Magnetic field: magnetic field B seen through Lorentz force on a moving charge, unit for I defined through force on a straight current, torque on a current loop in B field, magnetic dipoles in atoms and molecules, gyromagnetic ratio.

AMC14101 Numerical & Statistical Methods (4 0 0)

A). Numerical Methods:

Approximations and errors in computation and their evaluation – rounding off and truncation; Absolute, relative and percentage errors. Solution of non-linear algebraic and transcendental equations; Newton-Raphson, iterative, false position and bisection method; Generalized Newton's method for multiple roots. Finite difference operators and their relations, factorial notation of a polynomial, data smoothing. Newton-Gregory and Lagrange's interpolation formulae; Inverse interpolation by Lagrange's and iterative methods; Cubic spline. Numerical differentiation and integration – trapezoidal, Simpson and Weddle rules and Gaussian quadrature formula. Numerical solution of first order ordinary differential equations by Picard's, Taylor's, Euler's, modified Euler's, Runge – Kutta and Milnes methods; Solution of simultaneous first order and second order ordinary differential equations by Runge-Kutta and Milnes methods. Solution of boundary value problems by finite difference method. Numerical solution of PDE-Laplace's equation, wave equation, heat conduction equation.

Computer programming of the following: (i) N-R method (ii) iterative method (iii) method of false position, (iv) Lagrange's interpolation formula, (v) trapezoidal, Simpson and Weddle rules, (vi) Gauss elimination method, (vii) Gauss iteration method (viii) Euler and modified Euler methods (ix) Runge-Kutta and Milnes methods (x) Method of least square.

B) Statistical Methods:

Concept of frequency distribution, moments, skewness and kurtosis.

Probability: various approaches of probability-classical, frequency, statistical, subjective and axiomatic, theorems on probability, conditional probability, independence, Bayes theorem, random variable – discrete and continuous, distribution functions and their properties, probability mean and density function, mathematical expectation/moment generating function and its properties.

Probability distribution, Bernoulli's Binomial, Negative binomial, Poisson and Normal distribution.

Theory of least squares and curve fitting.

Correlation – simple, multiple and partial, regression lines, regression coefficients, multiple and partial correlation coefficients.

Test of significance: normal test, t-test, Chi-square test and f-test.

Introduction to non-parametric test.

Elements of statistical quality control, scope of practice session, computation of raw moments, central moments, coefficients of variations, coefficients of skewness and kurtosis, fitting of straight line, second degree parabola, power curve and exponential curve, computation of product moment correlation, multiple and partial correlation coefficient, and regression line, plane of regression, application of test of significance based on numerical data, mean chart, range chart and sigma chart.

Practical

ACC14222 Physical Chemistry Lab-I (0 0 3)

To determine the specific reaction rate of the hydrolysis of methyl acetate/ethyl acetate catalyzed by hydrogen ions at room temperature.

To study the effect of acid strength on the hydrolysis of an ester.

To compare the strengths of HCl and H₂SO₄ by studying the kinetics of hydrolysis of ethyl acetate.
 To study kinetically the reaction rate of decomposition of iodide by H₂O₂.
 To study the distribution of iodine between water and CCl₄.
 To study the distribution of benzoic acid between benzene and water.
 To prepare arsenious sulphide sol and compare the precipitating power of mono-, bi- and trivalent anions.
Viscosity, Surface Tension
 To determine the percentage composition of a given mixture (non interacting systems) by viscosity method.
 To determine the viscosity of amyl alcohol in water at different concentrations and calculate the excess viscosity of these solutions.
 To determine the percentage composition of a given binary mixture by surface tension method (acetone & ethyl methyl ketone).

ACC14223 Organic Lab-I (0 0 3)

Determination of M.P & B.P of organic compounds
 Detection of N, S, Cl, Br, I in organic compounds
 Qualitative analysis of functional groups
 Detection of aldehydes, ketone, carboxylic acids, amine, esters, phenols, amides
 Preparation of methyl salicylate, succinic anhydride, aspirin

APC94201 Electricity & Magnetism Lab (0 0 3)

Determination of Refractive index of a liquid by Abbe Refractometer.
 Study of Operational Amplifier applications.
 To verify the discrete atomic energy levels by Frank & Hertz experiment.
 Study of various Logic gates using diodes & transistors and IC.
 Determination of Susceptibility of paramagnetic solution by Quinck's tube.

AMC14201 Numerical & Statistical Methods Practical (0-0-3)

Numerical Methods; Numerical solution of non-linear algebraic and transcendental equations by Iteration Method, Newton-Raphson Method and Method of false position; Interpolation by Lagranges Method; Numerical Integration by Trapezoidal Rule, Simpson 1/3rd & 3/8th Rule and Weddles Rule; Numerical solution of ordinary differential equations by Eulers, Modified Eulers, Runge-Kutta and Milne's Predictor-corrector Method.

Statistical Methods: Preparation of frequency distribution table for discrete & continuous data, Ogive curves; Measures of central tendency, dispersion, skewness and kurtosis; Curve fitting of straight line, second degree polynomial, exponential and power curves; correlation and regression lines, multiple and partial correlation; Tests of significance of mean and variance based on one & two normal populations; Quality control (control Charts for mean & range).

V SEMESTER

Theory

ACC15125 Physical Chemistry – II (3 1 0)

Thermodynamics – I

First law of Thermodynamics. Heat capacity, heat capacities at constant volume and pressure and their relationship. Joule's law – Joule-Thomson coefficient and inversion temperature. Calculation of w, q, dU & dH for the expansion of ideal gases under isothermal and adiabatic conditions for reversible process.

Thermochemistry: standard state, standard enthalpy of formation – Hess's Law of heat summation and its applications. Heat of reaction at constant pressure and at constant volume. Enthalpy of neutralization. Bond dissociation energy and its calculation from thermo-chemical data, temperature dependence of enthalpy. Kirchhoff's equation.

Thermodynamics – II

Second law of thermodynamics: need for the law, different statements of the law. Carnot cycle and its efficiency, Carnot theorem. Thermodynamic scale of temperature.

Concept of entropy: entropy as a state function, entropy as a function of V & T, entropy as a function of P & T, entropy change in physical change, Clausius inequality, entropy as a criteria of spontaneity and equilibrium. Entropy change in ideal gases and mixing of gases.

Gibbs and Helmholtz functions; Gibbs function (G) and Helmholtz function (A) as thermodynamic quantities, A & G as criteria for thermodynamic equilibrium and spontaneity, their advantage over entropy change. Variation of G and A with P, V and T.

Third law of thermodynamics: Nernst heat theorem, statement and concept of residual entropy, evaluation of absolute entropy from heat capacity data.

Chemical Equilibrium

Equilibrium constant and free energy. Reaction isotherm and reaction isochore – Clapeyron equation and Clausius – Clapeyron equation, applications.

Phase Equilibrium

Derivation of Gibbs phase rule, phase equilibria of one component system – water and S systems.

Phase equilibria of two component system – solid-liquid equilibria, simple eutectic – Bi-Cd, pH-Ag systems,

Solid solutions – compound formation with congruent melting point (Mg-Zn) and incongruent melting point, (NaCl-H₂O).

Liquid – liquid mixtures – Ideal liquid mixtures, Raoult's and Henry's law. Non-ideal system-azeotropes – HCl-H₂O and ethanol – water systems.

Partially miscible liquids – Phenol-water, trimethylamine-water, nicotine-water systems. Lower and upper consolute temperature. Effect of impurity on consolute temperature.

Immiscible liquids, steam distillation.

Nernst distribution law – thermodynamic derivation, applications.

Electrochemistry

Electrical transport-conduction in metals and in electrolyte solutions, specific conductance and equivalent conductance, measurement of equivalent conductance, variation of equivalent and specific conductance with dilution.

Migration of ions and Kohlrausch law, Arrhenius theory of electrolyte dissociation and its limitations, weak and strong electrolytes, Ostwald's dilution law its uses and limitations. Debye-Huckel-Onsager's equation for strong electrolytes (elementary treatment only). Transport number, definition and determination by Hittorf method and moving boundary method.

Applications of conductivity measurements: determination of degree of dissociation, determination of K_a of acids, determination of solubility product of a sparingly soluble salt, conductometric titrations.

Buffers – mechanism of buffer action, Henderson-Hasselbach equation. Hydrolysis of salts.

ACC15126 Inorganic Chemistry – III (3 1 0)

Hard and Soft Acids and Bases (HSAB)

Classification of acids and bases as hard and soft. Pearson's HSAB concept, acid-base strength and hardness and softness. Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness and softness.

Metal-ligand Bonding in Transition Metal Complexes

Limitations of valence bond theory, an elementary idea of crystal-field theory, crystal field splitting in octahedral, tetrahedral and square planar complexes, factors affecting the crystal-field parameters.

Magnetic Properties of Transition Metal Complexes

Types of magnetic behaviour, methods of determining magnetic susceptibility, spin-only formula. L-S coupling, correlation of μ_s and μ_{eff} values, orbital contribution to magnetic moments, application of magnetic moment data for 3d-metal complexes.

Electron Spectra of Transition Metal Complexes

Types of electronic transitions, selection rules for d-d transitions, spectroscopic ground states, spectrochemical series, Orgel-energy level diagram for d^1 and d^9 states, discussion of the electronic spectrum of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex ion.

Thermodynamic and Kinetic Aspects of Metal Complexes

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability, substitution reactions of square planar complexes, Trans Effect.

ACC15127 Organic Chemistry – III (3 1 0)***Electromagnetic Spectrum : Absorption Spectra***

Ultraviolet (UV) absorption spectroscopy – absorption laws (Beer-Lambert law), molar absorptivity, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation. Concept of chromophore and auxochrome. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts. UV spectra of conjugated enes and enones. Infrared (IR) absorption spectroscopy – molecular vibrations, Hooke's law, selection rules, intensity and position of IR bands, measurement of IR spectrum, fingerprint region, characteristic absorptions of various functional groups and interpretation of IR spectra of simple organic compounds.

Spectroscopy

Nuclear magnetic resonance (NMR) spectroscopy.

Proton magnetic resonance (^1H NMR) spectroscopy, nuclear shielding and deshielding, chemical shift and molecular structure, spin-spin splitting and coupling constants, areas of signals, interpretation of PMR spectra of simple organic molecules such as ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromoethane, ethyl acetate, toluene and acetophenone. Problems pertaining to the structure elucidation of simple organic compounds using UV, IR and PMR spectroscopic techniques.

Gas Chromatography: Basic concepts

Organometallic Compounds

Organomagnesium compounds: the Grignard reagents-formation, structure and chemical reactions.

Organolithium compounds: formation and chemical reactions.

Organosulphur Compounds

Nomenclature, structural features, Methods of formation and chemical reactions of thiols, thioethers, sulphonic acids, sulphonamides and sulphaguanidine.

Heterocyclic Compounds

Introduction and preparation of simple heterocyclic compounds (furan, pyrrole, thiophene and pyridine)

CSR15101 Data Structure (3 0 0)

Basics of computer: structure and functioning, Memory, I/O devices. Secondary storage. Computer languages.

Operating systems: with DOS as an example.

Introduction to UNIX and WINDOWS.

Data processing, principles of programming. Algorithms and flowcharts.

Computer programming in FORTRAN / C / BASIC

Elements of the computer language, Constants and variables. Operations and symbols. Expressions.

Arithmetic assignment statement. Input and output. Format statement.

Termination statements. Branching statements such as IF or GO TO statement.

Logical variables. Double precision variables. Subscripted variables and dimension. DO statement. function and subroutine. common and data statements.

Programming in Chemistry

Computer codes for simple formula in chemistry such as Vander Walls equation, pH titration, kinetics, radioactive decay, lattice energy and ionic radii

Linear simultaneous equations to solve secular equations within the Huckel theory.

Elementary structural features such as bond lengths, bond angles, dihedral angles etc of molecules extracted from a data base such as Cambridge data base.

Use of Computer Programmes

Operation of a PC, run standard programmes and packages.

Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes.

Monte Carlo and Molecular dynamics. Programmes with data from physical Chemistry experiments.

Operation of the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO and Word processing software such as WORDSTAR / MS-WORD.

ACC15141 Introduction to Biochemistry (3 0 0)

Metal Storage Transport and Biomineralization: Ferritin, transferrin, and siderophores

Calcium in Biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins

Metalloenzymes: Zinc enzymes-carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase, peroxidase and cytochrome P-450. Copper enzymes – superoxide dismutase. Molybdenum oxotransferase enzymes- xanthine oxidase. Coenzyme vitamin B₁₂.

Metal-Nucleic Acid Interactions: Metal ions and metal complex interactions. Metal complexes-nucleic acids.

Metals in Medicine: Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

Practical

ACC15225 Physical Chemistry Lab -II (0 0 3)

Transition Temperature

1. Determination of the transition temperature of the given substance by thermometric/dilatometric method (e.g. $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}/\text{SrBr}_2 \cdot 2\text{H}_2\text{O}$).

Phase Equilibrium

1. To study the effect of a solute (e.g. NaCl, succinic acid) on the critical solution temperature of two partially miscible liquids (e.g. phenol-water system) and to determine the concentration of that solute in the given phenol-water system.

2. To construct the phase diagram of two component (e.g. diphenylamine-benzophenone) system by cooling curve method.

Thermochemistry

1. To determine the solubility of benzoic acid at different temperatures and to determine ΔH of the dissolution process.

2. To determine the enthalpy of neutralization of a weak acid/weak base versus strong base/strong acid and determine the enthalpy of ionization of the weak acid/weak base.

To determine the enthalpy of solution of solid calcium chloride and calculate the lattice energy of calcium chloride from its enthalpy data using Born Haber cycle.

ACC15226 Inorganic Chemistry Lab – II (0 0 3)

Volumetric Analysis

- Determination of acetic acid in commercial vinegar using NaOH.
- Determination of alkali content – antacid tablet using HCl.
- Estimation of calcium content in chalk as calcium oxalate by permanganometry.

Gravimetric Analysis

Analysis of Cu as CuSCN and Ni as Ni (dimethylglyoxime).

Synthesis and Analysis

Preparation of sodium trioxalato ferrate (III), $Na_3[Fe(C_2O_4)_3]$ and determination of its composition by permanganometry.

- Preparation of Ni-DMG complex, $[Ni(DMG)_2]$.
- Preparation of copper tetraammine complex. $[Cu(NH_3)_4]SO_4$.

Preparation of *cis*- and *trans*- bisoxalato diaqua chromate (III) ion.

ACC15227 *Organic Chemistry Lab- II* (0 0 3)

Stream Distillation of organic compounds.

Column Chromatography of dyes and pigments.

Qualitative Analysis

Analysis of an organic mixture containing two solid components using water, $NaHCO_3$, $NaOH$ for separation of compounds.

VI SEMESTER**Theory**

ACC16128 **Physical Chemistry – III** (3 1 0)

Elementary Quantum Mechanics

Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (no derivation) and its defects, Compton effect.

De Broglie hypothesis, the Heisenberg's uncertainty principle, Sinusoidal wave equation, Hamiltonian operator, Schrodinger wave equation and its importance, physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box.

Schrodinger wave equation for H-atom, separation into three equations (without derivation), quantum numbers and their importance, hydrogen like wave functions, radial wave functions, angular wave functions.

Molecular orbital theory, basic ideas – criteria for forming M.O from A.O, construction of M.O's by LCAO – H_2^+ ion, calculation of energy levels from wave functions, physical picture of bonding and antibonding wave functions, concept of σ , σ^* , π , π^* orbitals and their characteristics. Hybrid orbitals – sp , sp^2 , sp^3 ; calculation of coefficients of A.O.'s used in these hybrid orbitals.

Introduction to valence bond model of H_2 , comparison of M.O. and V.B. models.

Spectroscopy

Introduction: electromagnetic radiation, regions of the spectrum, basic features of different spectrometers, statement of the Born-Oppenheimer approximation, degrees of freedom.

Rotational, Vibrational and Electronic Spectra – basic concepts.

Photochemistry

Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus – Drapper law, Stark – Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes, quantum yield, photosensitized reactions – energy transfer processes (simple examples).

Physical Properties and Molecular Structure

Optical activity, polarization – (Clausius – Mossotti equation), orientation of dipoles in an electric field, dipole moment, induced dipole moment, measurement of dipole moment-temperature method and refractivity method, dipole moment and structure of molecules, magnetic properties- paramagnetism, diamagnetism and ferromagnetism.

Solutions, Dilute Solutions and Colligative Properties

Ideal and non-ideal solutions, methods of expressing concentrations of solutions, activity and activity coefficient.

Dilute solutions, colligative properties, Raoult's law of osmotic pressure and its measurement, determination of molecular weight from osmotic pressure. Elevation of boiling point and depression of

freezing point, Thermodynamic derivation of relation between molecular weight and elevation in boiling point and depression in freezing point. Experimental methods for determining various colligative properties. Abnormal molar mass, degree of dissociation and association of solutes.

Electrochemistry

Types of reversible electrodes – gas-metal ion, metal-metal ion, metal-insoluble salt-anion and redox electrodes. Electrode reactions, Nernst equation, derivation of cell E.M.F. and single electrode potential, standard hydrogen electrode-reference electrodes-standard electrode potential, sign conventions, electrochemical series and its significance.

Electrolytic and Galvanic cells – reversible and irreversible cells, conventional representation of electrochemical cells.

EMF of a cell and its measurements. Computation of cell EMF. Calculation of thermodynamic quantities of cell reactions (ΔG , ΔH and K), polarization, over potential and hydrogen overvoltage.

Concentration cell with and without transport, liquid junction potential, application of concentration cells, valency of ions, solubility product and activity coefficient, potentiometric titrations.

Definition of pH and pK_a determination of pH using hydrogen, quinhydrone and glass electrodes, by potentiometric methods.

ACC16129 Inorganic Chemistry –IV (3 1 0)

Organometallic Chemistry

Definition, nomenclature and classification of organometallic compounds. Preparation, properties, bonding and applications of alkyls and aryls of Li, Al, Hg, Sn and Ti, a brief account of metal-ethylenic complexes and homogeneous hydrogenation, mononuclear carbonyls and the nature of bonding in metal carbonyls.

Bioinorganic Chemistry

Essential and trace elements in biological processes, metalloporphyrins with special reference to haemoglobin and myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+} . Nitrogen fixation.

Inorganic polymers.

ACC16130 Organic Chemistry- IV (3 1 0)

Organic Synthesis *via* Enolates

Acidity of α -hydrogens, alkylation of diethyl malonate and ethyl acetoacetate. Synthesis of ethyl acetoacetate: the Claisen condensation. Keto-enol tautomerism of ethyl acetoacetate.

Carbohydrates

Classification, nomenclature and chemistry.

Amino Acids, Peptides, Proteins and Nucleic Acids

Fats, Oils and Detergents

Synthetic Dyes

Colour and constitution (electronic concept). Classification of dyes. Chemistry and synthesis of Methyl orange, Congo red, Malachite green, Crystal violet, Phenolphthalein, Fluorescein, Alizarin and Indigo.

Synthetic Polymers, Natural and synthetic rubbers.

CSR16102 Computer Networks (3 0 0)

Overview of data communication and networking, Network architecture; Physical layer communication: Signals, Media, Bits, Digital transmission; Circuit/packet switching, Error detection/correction techniques; Data link control and protocols, Medium access control: Pure/slotted ALOHA, CSMA/CD, CSMA/CA; Ethernet addressing and wiring; Internetworking: Architecture, IP addressing, Address binding with ARP; Datagram encapsulation and fragmentation, Link state and distance vector routing, Dijkstra's/Bellman-Ford Algorithms, IPv6 Internet protocols, UDP and TCP, TCP segment format, Protocol ports, ICMP and

error handling, Network applications: Client/Server concepts, Socket API, DNS, Electronic mail, HTTP and WWW including HTML.

HSC36107 Communication Skills (3 1 0)

The Process of Communication, barriers to communication, overcoming the barriers to communication, effective verbal communication, non-verbal communication. Speaking and listening, listening strategies, effective speaking, social interaction, professional interaction, academic speaking and listening skills, oral presentation: seminar presentation and team presentation. CV/Resume writing, job application, proposals, reports, writing articles and research papers.

Practical

ACC16228 Physical Chemistry Lab.-III (0 0 3)

Electrochemistry

- (a) To determine the strength of the given acid conductometrically using standard alkali solution.
- (b) To determine the solubility and solubility product of a sparingly soluble electrolyte conductometrically.
- (c) To study the saponification of ethyl acetate conductometrically.
- (d) To determine the ionization constant of a weak acid conductometrically.
- (e) To titrate potentiometrically the given ferrous ammonium sulphate solution using $\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ as titrant and calculate the redox potential of $\text{Fe}^{++}/\text{Fe}^{+++}$ system on the hydrogen scale.

Refractometry, Polarimetry

- a) To verify law of refraction of mixtures (e.g., of glycerol and water) using Abbe's refractometer.
- b) To determine the specific rotation of a given optically active compound.

Molecular Weight Determination

- a) Determination of molecular weight of a non-volatile solute by Rast method/Bechmann freezing point method.
- b) Determination of the apparent degree of dissociation of an electrolyte (e.g., NaCl) in aqueous solution at different concentrations by ebullioscopy.

Colorimetry

To verify Beer – Lambert law for $\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$ and determine the concentration of the given solution of the substance.

ACC16229 Inorganic Chemistry Lab.- III (0 0 3)

Colorimetry, (a) Job's method (b) Mole-ratio method
Adulteration – Food Stuffs., Effluent analysis, water analysis, Solvent Extraction
Separation and estimation of Mg(II) and Fe(II))

Ion Exchange Method

Separation and estimation of Mg(II) and Zn(II).

ACC16230 Organic Chemistry Lab. –III (0 0 3)

Synthesis of Organic Compounds

Preparation of iodoform from ethanol and acetone

- a) Aromatic electrophilic substitution
Preparation of p-bromoacetanilide
Preparation of 2,4,6-tribromophenol
- b) Diazotization/coupling
Preparation of methyl orange and methyl red
- c) Oxidation
Preparation of benzoic acid from toluene
- d) Reduction
Preparation of aniline from nitrobenzene

VII SEMESTER

Theory

ACC31131

Physical Chemistry –IV

(3 1 0)

Quantum Theory: Techniques and applications, Exact solution, particle in a box, harmonic oscillation, tunneling, wave function. Time dependent and time independent perturbation theories.

Electronic structure of atoms: electronic configuration, RS terms and schemes, Slater Condon parameters, spin orbit coupling, Zeeman splitting, method of self consistent field and the virial theorem. Molecular structure, molecular orbital Huckel approximation, Extended Huckel theory, Self consistent field calculation.

Equilibrium Thermodynamics: Review of the laws of thermodynamics, Free energy and chemical equilibria, van't Hoff's isotherm and isochore, Gibbs-Helmholtz equation, Ellingham diagram-method of free energy determination; Non ideal systems, Thermodynamics of solutions, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Statistical Thermodynamics: Distribution of molecular states, internal energy and entropy, canonical partition function, thermodynamic relations; Determination of mean energies, heat capacities, residual entropies, equilibrium constants. FD statistics, BE statistics and their applications in electrons in metals, photons. BE condensation.

Chemical Kinetics: Theories of reaction rates, kinetics and thermodynamic control of reactions. Reactions in solutions, Effect of pressure, dielectric constant and ionic strength; kinetic of enzyme catalysed reactions, fast reactions; Theories of unimolecular reactions and catalysis

ACC31132

Organic Chemistry – V

(3 1 0)

Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π molecular orbitals, annulenes, antiaromaticity. Bond weaker than covalent- addition compound, crown ether complexes and cryptands, inclusion compounds, cyclodextrins. Phase transfer catalysis.

Stereochemistry: Conformational analysis of cycloalkanes, decalin, effect of conformation on reactivity, Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (Biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

Reaction Mechanism: Structure and Reactivity. Types of mechanism, types, of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbonions, free radicals, carbenes and nitrenes. Aliphatic nucleophilic substitution: The S_N2 , S_N1 mixed S_N1 and S_N2 and SET mechanism. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements.

ACC 31133 Inorganic Chemistry –V (3 1 0)

Metal-Ligand Bonding: Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square-planar complexes, π -bonding & molecular orbital theory.

Reaction Mechanism of Transition Metal Complexes: Energy profile of a reaction, reactivity of metal complexes, inert & labile complexes, kinetic applications of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and evidences in favour of conjugate mechanism, anation reactions, reactions without metal-ligand bond cleavage. Substitution reaction in square planar complexes, the trans effect, mechanism of substitution reaction, redox reactions, electron transfer reaction, outer sphere reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Metal-ligand Equilibria in Solution: Step-wise and overall formation constants and their interaction, trends of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry .

ACC31134 Analytical Chemistry- I (3 1 0)

Statistical tests and error analysis: Accuracy, precision, classification of errors, minimisation of errors, significant figures and computation, mean deviation and standard deviation, Gaussian distribution, mean value statistics.

Sampling and sample treatment: Factors involved in effective sampling, good samples; representative and homogeneous; the binomial distribution, samples of mixtures, physical separations in sample preparation, preconcentration and predilution.

Gravimetric Analysis: Theory of gravimetric analysis: introduction, solubility, solubility product, common ion effect, precipitation methods, the colloidal state, super-saturation, precipitate formation, co-precipitation, condition of precipitation, precipitation from homogeneous solution, purity of precipitates. Washing of precipitates, ignition of precipitates, thermogravimetric analysis.

Titrimetric Analysis: Acid-base titrations: Classification, theory of acid-base titrations, neutralisation indicators, mixed indicators, universal indicators, neutralisation curves, choice of indicators in neutralisation reactions. Complexometric titrations: Stability of complexes, factors influencing the stability of complexes, stability constants of EDTA complexes, titration curves, selectivity, masking and demasking agents, metal ion indicators. Precipitation titrations: Theory of precipitation reactions, determination of end points in precipitation reactions.

Oxidation-reduction titrations: Theory, change of electrode potential during the titration of a reductant with an oxidant, formal potentials, detection of end points in oxidation-reduction titrations, titrations in non-aqueous media.

Electroanalytical methods: Theory of electrogravimetric analysis, electrode reactions, overpotential, completeness of deposition, electrolytic separation of metals with controlled cathode potential.

Potentiometry: Reference electrodes, indicator electrodes, ion-selective electrodes, instrumentation and measurement of cell emf, potentiometric titrations. Amperometric titrations.

ACC31147 Chemistry of materials (3 0 0)

Glasses, ceramics, composites and nanomaterials:

Structure of glass, glass formers and glass modifiers. Applications of glass. Ceramic structure, mechanical properties, clay and clay products. Microscopic composites- dispersion strengthened and particle reinforced, fibre reinforced composites, macroscopic composites. Nanocrystalline phase, preparation, properties and applications.

Thin films and Langmuir- Blodgett Films: Preparation techniques. Langmuir-Blodgett film, growth techniques, properties and applications of thin film.

Liquid crystals: Mesomorphic behaviour, thermotropic liquid crystals, nematic and smectic mesophases. Optical and dielectric properties of liquid crystals. Lyotropic phases and their description of ordering.

High T_C materials: Perovskites. Properties and preparation of 1-2-3 and 2-1-4 materials. Properties dependent of temperature. Application of high T_C materials.

Organic solids, fullerenes and molecular devices: Conducting organic materials and Fullerenes-preparation and properties. Molecular rectifiers and transistors. Optical storage devices, sensors. Nonlinear optical materials

Practical

ACC31231 Chemistry Practical I (0 0 3)

Special identification tests for mixture of acid radicals; qualitative analysis of less common elements- TI, Mo, W, Ti, Zr, Th, V, U (two metal ion in cationic/anionic forms).

Volumetric analysis: redox, complexometric and precipitation titration.

Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods, Ore analysis.

Determination of Iodine and Saponification values of an oil sample.

ACC31232 Chemistry Practical II (0 0 3)

TLC Analysis of organic compounds. Identification of functional groups by IR Spectroscopy

Synthesis of Ester, Alcohol, Ketones (Jones Reduction)

ACC32233 Chemistry Practical III (0 0 3)

Adsorption: To study surface tension – concentration – relationship for solutions (Gibbs equation)

Phase Equilibria: Determination of congruent composition and temperature of a binary system. To construct the phase diagram for three component system.

Chemical Kinetics: Determination of the effect of (a) change of temperature (b) change of concentration of reactants and catalyst and (c) ionic strength of the media on the velocity constant of hydrolysis ester/ ionic reaction. Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.

Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)

Solutions: Determination of molecular weight of non- volatile and non- electrolyte/ electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry: *Conductometry*: Determination of solubility and solubility product of sparingly soluble salts (e.g. PbSO_4 , BaSO_4) conductometrically. *Potentiometry / pH metry*: Determination of the strength of strong and weak acid in a given mixture using a potentiometer / pH meter.

VIII SEMESTER

Theory

ACC32135 Physical Chemistry – V (3 1 0)

Surface Chemistry: Adsorption, catalytic activity, micelles, macromolecules.

Theory of electrolytic conductance - Debye-Huckel theory of strong electrolytes - Debye-Huckel-Onsager equation - validity of DHO equation - deviation of DHO, migration of ions, transport number in simple electrolytes and mixtures - abnormal transport number. Activity coefficients of electrolytes - ionic

strength, Debye-Huckel limiting law, modifications of DHLL, qualitative test of DHLL, verification of DHLL, ion association, fraction of association, association constant, equilibria in electrolytes - dissociation constant, activity coefficient and solubility measurements. Applications of conductance measurements.

Diffusion: Fick's Law of steady state diffusion, diffusion coefficient, relation between diffusion and mobility.

Galvanic cells: Cells with and without transference, liquid junction potential and its determination, Donnan membrane equilibrium, Applications of EMF measurements - solubility and solubility product, pH and its measurement, Temperature coefficient of EMF and determination of ΔG , ΔH and ΔS .

Non equilibrium thermodynamics: Thermodynamic criteria for non-equilibrium states, entropy production, flow, irreversible processes. Onsager reciprocal relations. Electrokinetic phenomena. Diffusion, Electric conduction, irreversible thermodynamics for biological systems. Coupled reactions.

ACC32136 Organic Chemistry VI (3 1 0)

Aliphatic Electrophilic Substitution: Bimolecular mechanism S_E2 and S_E1 . The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution: The S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

Pericyclic Reaction: Molecular orbital symmetry, Frontier orbitals of ethylene 1,3 butadiene, 1,3,5, hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motion, $4n$, $4n+2$ and allyl systems. Cycloadditions – antarafacial and suprafacial addition, $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, 1,3, dipolar cycloadditions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3, and 5,5 sigmatropic rearrangements. Ene reaction.

ACC32137 Inorganic Chemistry –VI (3 1 0)

Nuclear Chemistry: Radioactivity : General characteristics of radioactive decay, Decay kinetics, α , β decay, γ emission, artificial radioactivity. Nuclear Reactions: Elastic, inelastic, Photoneuclear, radioactive capture, evaporation, spallation, Fragmentation, Transfer reactions. Nuclear fission and fission; Nuclear Reactors: Classification of reactors, reactor power, and application of radioactivity, nuclear waste Management.

Metal Clusters: Metal carbonyl and halide clusters, compounds with metal-metal multiple bond.

Isopoly & heteropoly acids & salts.

Organometallic Chemistry: Metal π - complexes, metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls, bonding & structural elucidation, reactions of metal carbonyls, preparation bonding structure & important reactions of metal nitryl, dinitrogen & dioxygen complexes, tertiary phosphine complexes.. chemistry of boranes and phosphazenes.

ACC32138 Introduction to Group Theory (3 0 0)

Symmetry elements and symmetry operations, definition of group, subgroup, relations between orders of a finite group and its subgroup. Schonflies symbols, matrix representations of symmetry operations, point groups, irreducible representations and character tables.

Orthogonality theorem and its importance.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization, classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy. Woodward-Hoffman rules.

CSR16101 Data Base Management System (3 1 0)

Introduction and Overview of a DBMS: Purpose of Database Systems, View of Data, Data Models, DDL, DML, Transaction Management, Storage Management, Database Administrator, Database Users, Overall System Structure; Entity-Relationship Model: Basic Concepts, Design Issues, Mapping Constraints, Keys, ER-Diagram, Weak Entity Sets, Extended ER-Diagram, Reduction of ER-Schema to Tables; Relational Model Concepts: Structure of Relational Databases, Relational Algebra, Tuple Relational Calculus, Domain Relational Calculus, Extended Relational-Algebra Operations, Modification of the Database, Views; Other Data Models: Hierarchical Data Model, Network Data Model, Unifying Data Model, Frame-memory Model; Structured Query Language; Integrity Constraints: Domain Constraints, Referential Integrity, Assertions, Triggers, Functional Dependencies; Relational Database Design: Decomposition, Normalization; Transactions and Concurrency Control: Transaction Concepts, Transaction State, Concurrent Executions, Serializability, Recoverability, Lock-Based Protocols, Timestamp-Based Protocols, Deadlock Handling; Basics of Database File Organization: File Organization, Organization of Records in Files, Data Dictionary Storage; Basics of Query Processing: Steps in Query Processing.

Practical

ACC32239 Computer Application in Chemistry Lab (0 0 3)

C++ programming: Classes and objects, Arrays of objects, Passing objects to member functions. Function overloading, Friend functions, Passing objects to friend functions Member functions/Friend functions returning objects. Pointer: Accessing data members and member functions using pointers. Constructors and Destructors: constructors, parameterized constructors, overloaded constructors, Copy constructors, Dynamic constructors; destructors. Operator Overloading: Overloading of unary operators such as minus, increment operator, decrement operator etc.; Overloading of binary operators such as +, * etc.; overloading of operators such as >>, << etc. Type Conversions: Basic type to class type, Class type to basic type, one class type to another class type. Inheritance: Single Inheritance, Multiple Inheritance, Hierarchical Inheritance, Multilevel Inheritance and Hybrid inheritance. Constructors in Derived classes, Polymorphism: Run time polymorphism- Virtual functions. Console oriented I/O operations: using ios class functions and flags, Manipulators, User-defined output functions. File Processing: Sequential files, Random Files, Accessing files using class objects, Updating a file Templates: Function Templates, Class Templates, Error Handling.

JAVA programming: Simple programs in JAVA

DBMS: Development of database using suitable DBMS packages

ACC32234 Chemistry Practical IV (0 0 3)

Ion exchange separation of oxidation states of vanadium; Bromination of Cr (acac)₃.
 Synthesis and characterization of metal complexes of DMSO
 Synthesis of cis- and trans- [Co (en)₂Cl₂]⁺
 Preparation of Cr (III) complexes: [Cr(H₂O)₆] NO₃.3H₂O, [Cr(H₂O)₄Cl₂]Cl.2H₂O, [Cr(en)₃]Cl₃, Cr(acac)₃.
 Preparation of triphenylphosphine Ph₃P and its transition metal complexes
 Preparation of cis and trans complexes of Cu with glycine

ACC33235**Chemistry Practical V****(0 0 3)**

Chemical Kinetics: Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.
 Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
 Electrochemistry: Determination of the activity coefficient of zinc ions in the solution of 0.002 M Zinc sulphate using Debye Huckel's limiting law.
 To study the effect of solvent on the conductance of AgNO₃/ acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
 Determination of temperature dependence of EMF of a cell.
 Determination of thermodynamic constants ΔG, ΔS and ΔH for the reaction by EMF method.
 Determination of activity and activity coefficients of electrolytes.
 Determination of corrosion rate of steel in acid medium by gravimetric method and electrochemical method.
 Viscosity: Determination of molecular weight of a polymer
 Adsorption: Acetic acid on charcoal.
 Thermodynamics: Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.
 Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution.

IX SEMESTER**Theory****ACC33140****Solid State Chemistry and Photochemistry****(3 0 0)**

Crystal Structure: Crystalline solids, crystal systems point groups: methods of characterising crystal structure - Powder x-ray diffraction, electron and neutron diffraction; types of close packing - hcp and ccp, packing efficiency, radius ratios; structure types -NaCl, ZnS, Na₂O, CdCl₂, wurtzite, nickel arsenide, CsCl, CdI₂, rutile and Cs₂O, perovskite ABO₃, K₂NiF₄, spinels. Defects - colour centers – reactivity,optical properties.
 Preparative methods: Solid state reaction, precipitative reactions, sol-gel route, precursor method, ion exchange reactions, intercalation / deintercalation reactions, glasses and thin film preparation..
 Electrical properties: Development of free electron theory to band theory of solids -metals and their properties; semiconductors - extrinsic and intrinsic, Hall effect; insulators - dielectric, ferroelectric, pyroelectric and piezoelectric properties and the relationship between them. Ionic conductivity
 Magnetic properties: Dia, para, ferro, ferri, and antiferro magnetic types -selected magnetic materials such as spinels, garnets and perovskites.
 Superconductivity: Theory, discovery and recent high T_c materials.
 Photochemistry: Photochemical reactions; determination of reaction mechanism; photochemistry of alkenes, carbonyl compounds and aromatic compounds. reactions of anilides and Photo-Fries rearrangement. Photochemistry of vision. Photosynthesis.

ACC33142 Analytical chemistry –II (Instrumental methods) (3 0 0)

Chromatographic methods of separation;
Electronic spectroscopy: Atomic, molecular and photoelectron
Microwave Spectroscopy;
Vibrational Spectroscopy: IR and Raman;
Magnetic Resonance spectroscopy: NMR, ESR, Nuclear Quadrupole resonance;
Mass spectroscopy
X-ray methods of analysis: XRD, XRF
Thermal Analysis: DTA, DSC, TG, DMA
Electrochemical techniques: Ion selective electrodes Voltammetry: Current-voltage relationship.,
Polarographic methods

HSC21103 Scientific Writing (2 2 0)

To receive and interpret written information: academic texts; journals and reference materials; manuals and laboratory instruction sheets; graphical information, viz. maps, tables, charts, graphs, diagrams, flow-charts, sketches, plans and statistical data.

Understanding interactive writing process and scientific writing with word, sentence and paragraph sense.
Writing physical descriptions, writing instructions and report; defining, describing processes; writing narratives, classifications, explanations; hypothesis, prediction and conclusion; generalizing and exemplifying; using graphical information and using thought connectors.

Note taking; outlining, paraphrasing, summarizing and writing abstracts; organizing references and writing assignments and revision of grammar.

ACE33143 Surface Chemistry and Catalysis (3 0 0)

Surface phenomena: Surface notation, clean and stepped surfaces; reconstruction, structure of adsorbate layers molecular chemisorption, surface energy, nucleation and growth, contact angle and adhesion, heat of adsorption, entropy and isotherms.

Surface vibrations: measurements, diffusion, desorption, surface chemical bond, chemisorption, thermal activation and precursor states.

Surface reactions: General aspects, coadsorption, poisoning and promotion effects, model reactions, detection of adsorbates on surfaces. High pressure catalytic reaction on single crystal surface. Surface modification.

Chemistry of bimetallic surface: Surface alloys, surface segregation and faceting. Determination of surface structure and chemical composition. Growth modes and study of metal over layers on single crystal surfaces. Chemical, electronic and catalytic properties of bimetallic surface.

Basic principles of catalysis: adsorption isotherms, surface area pore size and acid strength measurement. Enthalpy and entropy of adsorption: interpretation of chemisorptions based on the structure and the nature of the solid – solid state theories – role of defects in catalysis.

Kinetic of surface reactions: rate determining step, various types of reaction, simple, parallel and consecutive reactions.

Selection, preparation and evaluation of catalysts – test reaction, promoters, carriers and stabilizers.

Mechanisms of selected reactions: hydrogenation and dehydrogenation reaction – dehydration of alcohols, olefin hydrogenation, decomposition of nitrous oxide, oxidation of CO- ketonization of carboxylic acids, cracking of hydrocarbons.

Electrocatalysis and Photo catalysis: Solid liquid interfaces.

Techniques in catalysis.

ACE33144 Organic Synthesis (3 0 0)

Organometallic reagents: Principle, properties and applications of the compounds of the following in organic synthesis with mechanistic details: Li, Mg, Hg, Cd, Zn, Ce, Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti, S, Si, B and I.

Oxidation: Different oxidative processes, Oxidation of hydrocarbons, alcohols, carbonyl compounds, amines.

Reduction: Different reductive processes, Reduction of hydrocarbons, carbonyl compounds, nitro group containing compounds.

Protecting groups: Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

Ring synthesis: Saturated heterocycles, synthesis of 4-, 5- 6-membered rings, aromatic heterocycles in organic synthesis.

Synthesis of some complex molecules: camphor, cortisone..

ACE33145 Advanced Electrochemistry (3 0 0)

Electrodes: Electrified interface, Electrical double layer and its determination, current-voltage curves - reversible and irreversible electrode processes - factors contributing to the decomposition voltage - different kinds of overvoltage -hydrogen and oxygen overvoltage. Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants - Tafel equation, electrocapillarity , potential of zero charge, pzc of solid electrodes, polarization: types of polarization, the charge transfer resistance, kinetics of hydrogen evolution reaction.

Mechanism of electrode processes: Multielectron processes, chemical reactions initiated by electron transfer, standard mechanistic schemes.

Quantum aspects of charge transfer at electrodes – solution interfaces, quantization of charge transfer, tunnelling.

Semi conductor interfaces, Electro-catalysis, Bio-electrochemistry,

Electron transfer in homogeneous system and in heterogeneous system.

Electrosynthesis: Reductive elimination reactions, Kolbe's Hydrocarbon synthesis. Industrial processes: electroplating, anodization, Al production, electroorganic and electroinorganic syntheses, electrosynthesis of some industrial chemicals

ACE-33151 Bioinorganic Chemistry (3 0 0)

Symmetry elements and symmetry operations, definition of group, subgroup, relations between orders of a finite group and its subgroup. Schonflies symbols, matrix representations of symmetry operations, point groups, irreducible representations and character tables.

Orthogonality theorem and its importance.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization, classification of normal vibrational modes, selection rules in vibrational and electronic spectroscopy. Woodward-Hoffman rules.

ACE-33153 Bioorganic and Medicinal Chemistry (3 0 0)

Mechanism of enzyme action: Typical enzyme mechanism for ribonuclease, lysozyme, chemical models and mimics for enzymes, receptors, peptides, carbohydrates and other bioactive molecules. Design, synthesis and evaluation of enzyme inhibitors.

Enzyme catalysed reactions: Carboxylation and decarboxylation, Isomerization and rearrangement.

Drug design: Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, structure-activity relationship, mechanism of drug action.

Classification of drugs: Based on structure or pharmacological basis with examples. Antineoplastic agents, cardiovascular drugs, local anti-infective drugs, psychoactive drugs, antibiotics.

Synthesis: Synthesis of important drugs.

Modelling: Molecular modelling, conformational analysis.

Practical

ACC33236 Chemistry Practical VI (0 0 3)

Chemical Kinetics: Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.

Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

Electrochemistry: Determination of the activity coefficient of zinc ions in the solution of 0.002 M Zinc sulphate using Debye Huckel's limiting law.

To study the effect of solvent on the conductance of AgNO_3 / acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.

Determination of temperature dependence of EMF of a cell.

Determination of thermodynamic constants ΔG , ΔS and ΔH for the reaction by EMF method.

Determination of activity and activity coefficients of electrolytes.

Determination of corrosion rate of steel in acid medium by gravimetric method and electrochemical method.

Viscosity: Determination of molecular weight of a polymer

Adsorption: Acetic acid on charcoal.

Thermodynamics: Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.

Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution.

ACC33237 Chemistry Practical VII (0 0 3)

Quantitative Analysis: Estimation of amines/ phenols using bromate bromide solution / or acetylation method.

Organicsynthesis:Dryingofsolvents:Ethanol,Benzene,Chloroform.Synthesisofcyclohexylidencyanoacetates , and reduction thereof. Synthesis using phase transfer catalyst., Reduction: Using supported reducing agents

ACC33238 Chemistry Practical VIII (0 0 3)

Thermal analysis: Thermal decomposition of calcium oxalate, copper sulphate, calcium sulphate hydrate in cement.

Electrogravimetric analysis: Separation and determination of nickel and cobalt

Atomic Absorption spectroscopy:Determination of Zn and Cu

Flame photometry: Determination of Na, Ca, and K

UV-Vis spectrophotometry: Determination of As, Fe, Cr

IR spectrophotometry: Sample preparation, identification of functional groups.

X SEMESTER

Theory

ACC34146 Applications of Spectroscopy in Organic and in Inorganic Chemistry (3 1 0)

Nuclear Magnetic Resonance Spectroscopy: NMR phenomenon, spin 1/2 nuclei, ^1H , ^{13}C , ^{19}F and ^{31}P , Zeeman splitting, Boltzmann distribution, effect of magnetic field strength on sensitivity and resolution. ^1H -NMR, chemical shift, anisotropic effects, chemical and magnetic equivalence, coupling constants. Karplus relationship of J on dihedral angle, first order splitting patterns and structure correlation. Second order effects on the spectrum, AB, AMX, AA'BB' spin systems, simplification of second order spectra. High field NMR, double irradiation, selective decoupling, chemical shift reagents. ^{13}C satellites. - ^{13}C -NMR, natural abundance, sensitivity. Introduction to FT technique, relaxation phenomena, NOE effects, ^{13}C chemical shifts and structure correlations, off-resonance spectrum. - Dynamic processes by NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems), examples from few organometallic systems. Significance of coalescence temperature. - Introduction to ^{31}P and ^{19}F NMR.

Infrared and Raman spectroscopy: Vibrational modes, group frequencies of organic, inorganic and organometallic systems, factors affecting the group frequencies, study of hydrogen bonding effects, vibrational spectra of ionic, coordination and metal carbonyl compounds.

Mass spectrometry: Basic principle, ionization methods, isotope abundance, molecular ions, fragmentation processes of organic molecules and deduction of structural information, high resolution MS, introduction to soft ionization techniques and illustrative examples in macromolecular and supramolecular chemistry.

Electronic spectroscopy: Electronic levels and types of electronic transitions in organic, inorganic and organometallic systems, solvent effects, effect of extended conjugation, Woodward-Fieser rules for calculation of absorption maximum, stereochemistry and electronic absorption.

ESR spectroscopy: ESR phenomenon, introduction to the ESR spectra of organic free radicals and ion radicals, transition metal complexes, application of spin traps.

ACE34148 Organometallic Chemistry (3 1 0)

Introduction: Historical background of organometallics.

Classification, nomenclature, characteristics of organometallic compounds.

Organometallic compounds of main Group elements: Introduction, general characteristics, stability, routes to MC bond formation, structural aspects, cyclopentadienyl complexes of main group elements.

Organometallic compounds of transition metals: σ -bonded and π -bonded organometallics, metallocenes, organometallic compounds of lanthanides & actinides, metal carbonyls.

Fluxional Organometallic Compounds:Some examples of non rigid molecules in different coordination geometries, classification of fluxional organometallic compounds.

MSc (Chemistry), 5 year integrated

Indian School of Mines

Organometallic in Catalysis: Hydrogenation and dehydrogenation, hydrosilation, isomerisation, carbonylation, hydroformylation, Heck-reaction. Allylic alkylation, cyclopropanation and polymerisation of olefins (Ziegler-Natta catalyst), Monsanto process, Waker process, Fisher-Tropsch process, enantio selective reactions.

ACE34150 Electron, Nuclear and Radiation Spectroscopy (3 1 0)

Electron spectroscopy: Basic principle, classification of various spectroscopies.

Photoelectron spectroscopy: experimental methods-electron energy analysis-photon sources -- UV, X-ray, synchrotron, theory, angular dependence-cross section and its determination-valence and core photoemission - Koopmans' theorem-quantum chemical methods-final state effects - supersonic molecular beam spectroscopy - coincidence studies, photoelectron diffraction, band structure, holography, circular dichroism.

Electron energy loss spectroscopy: Franck and Hertz experiment -- instrumentation -selection rules-theory - studies on molecules - surface states - high resolution spectroscopy - adsorption and catalysis -applications.

Auger electron spectroscopy: introduction - instrumentation - classification of various transitions-quantization- applications-Auger microscopy.

Radiation Sources: Fast electron sources, heavy particle sources, sources of electromagnetic radiation, neutron sources.

Radiation Interactions: Interaction of heavy charged particles with matter, energy loss characteristics, particle range, range straggling and damage profiles, nuclear and electronic stopping powers, Interaction of fast electrons and transmission curves, interaction of gamma photons : photoelectric absorption, Compton scattering and pair production, gamma ray attenuation, interaction of neutrons, neutron cross sections.

Radiation Spectroscopy: Study of nuclear states, gamma ray spectroscopy with scintillation and HPGe detectors, Compton suppression, Particle - gamma coincidences, angular correlations and lifetime measurements. Secondary ion mass spectroscopy, Rutherford back scattering and resonant scattering, particle induced x-ray emission, nuclear reaction analysis.

Nuclear Processes as Chemical Probes: Mossbauer spectroscopy, positron annihilation lifetime spectroscopy, perturbed angular correlations of gamma rays.

ACE34154 Waste Utilization (3 1 0)

Waste: Types of waste, Hazardous waste, Radioactive waste. Lethal dose, Tolerance limit.

Solid Waste: Waste from thermal power Plant. Silica Fumes – Characterization and utilizations. Flyash – Genesis, coal combustion mechanism, different types of combustors (brief) PFC, FBC, CFBC, PFBC – implications of combustion process and genesis of ash. Characterization of Ash: Particle size distribution, chemical composition, Mineralogy, morphology of flyash. Use of fly ash in concrete / building material, in paint. Extraction of valuable elements present in flyash, use of flyash in agriculture, use of flyash to increase water holding capacity. Phenol removal using flyash. Rice husk ash – Recovery of amorphous silica and use in concrete.

Liquid waste: Effluents from coke oven – Processing of valuable materials. Effluents from phenol plant. recovery of phenols. Effluents from plants dealing with inorganic chemicals.

Metal recovery: Recovery of metals like Cr, Ni, V etc from electroplating wastes and spent catalysts

ACE34155 Science of Corrosion & Corrosion Control (3 1 0)

Definition of corrosion, economic aspects of corrosion , theories of corrosion.

Factors affecting corrosion. Kinetics of corrosion. Evan's diagram. Thermodynamics of corrosion-Pourbaix diagram. Forms of corrosion. Corrosion testing techniques

Evaluation of corrosion effect: XRD, ESCA, FTIR and surface techniques.

Corrosion prevention: modification of materials, corrosion inhibitors, protective coatings, Cathodic and anodic protection. Corrosion problems in industries.

ACE34152 Electrochemical Energy system (3 1 0)

Basic Principles of Electrochemical Engineering: Thermodynamics and kinetics of electrochemical systems, modeling of electrochemical systems, electrochemical analytical methods, fundamentals of typical electrochemical energy systems (batteries, fuel cells, solar system).

Fuel Cells Technology: alkaline fuel cells, phosphoric acid fuel cell, molten carbonate fuel cells, solid oxide fuel cells, polymer electrolyte fuel cells; cell components, thermodynamics and kinetics, operation and performance, applications.

ACE34149 Chemistry of Macromolecules (3 1 0)

Basic concepts: Classification, nomenclature, molecular weight and distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships. Chain structure and configuration, conformation of the polymer chain (freely jointed chain and other models).

Types of polymers: electrically conducting, fire resistant, liquid crystal polymers.

Methods of determination of molecular mass: Osmometry, viscometry, diffusion and light scattering methods. Distribution, size and shape of macromolecules. Intrinsic viscosity, Mark-Houwink relationship.

Thermodynamics of polymer solutions: Molecular motion (reptation, self-diffusion, Rouse-Bueche theory and de Gennes reptation model), Glass transition temperature (theories and methods of determination), Rubber elasticity - concepts, thermodynamic equations of state, theories.

Polymerisation reaction: Kinetics, mechanism and methods.

Step (condensation) polymerization: Description, Reactivity, Functional Groups -kinetic and thermodynamic considerations.

Chain polymerization: effect of substituents, structural arrangement of monomer units, molecular weight, chain transfer and termination. Factors affecting polymerization, methods of polymerisation- living polymerisation by atom - transfer-radical-polymerisation (ATRP).

Cationic chain polymerization: Initiation, propagation and termination, kinetics and energetics. Anionic

polymerization: Chain copolymerisation, determination of composition, specific copolymers, ring-opening polymerisation.

Ziegler-Natta polymerization, traditional and metallocene catalysts. Control of stereochemistry of polyolefins and polycyclo-olefins. Metathesis polymerisation - mechanism of polymerisation - synthesis of polyacetylenes - ring - opening - metathesis - polymerisation (ROMP) - synthesis block-graft copolymers- applications of metathesis polymerisation.

Mechanical properties and methods of determination.

Selected commercial polymers and applications; fibre reinforced plastics.