COURSE STRUCTURE

Sem.	Course No.	Courses	L T P	Credit Hr.
I	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			
	ACC32131	Chemistry Practical – I	0 – 0 – 3	03
	ACC32132	Chemistry Practical – II	0 – 0 – 3	03
	ACC32133	Chemistry Practical – III	0 – 0 – 3	03
		Total	15– 4 – 9	43

Sem.	Course No.	Courses	L T P	Credit Hr.
II	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
	AMC32102	Object Oriented Programming	3 -0 - 0	06
	Practical etc			
	ACC32234	Chemistry Practical – IV	0 – 0 – 3	03
	ACC32235	Chemistry Practical – V	0 – 0 – 3	03
	AMC32202	Object Oriented Programming Lab	0 -0 - 2	02
	ACC32239	Computer applications in Chemistry Lab	0 – 0 – 3	03
	ACC32602	Term paper	0 – 0 – 0	02
		Total	15 – 3 – 11	46
	Summer Training			
	ACC329 01	Summer Training Project (3 weeks)		

Sem.	Course No.	Courses	L T P	Credit Hr.
III	Theory			
	Core Courses			
	ACC-33140	Solid State Chemistry and Photochemistry	3 – 0 – 0	06
	ACC-33141	Introduction to Biochemistry	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 (Any one)			
	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
	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.
IV	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	45

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I 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 viral 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, Ellihgham 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, annulenes, antiaromaticity, addition compound, crown ether complexes and cryptands, inclusion compounds, cyclodextrins. Phase transfer catalysis.
Stereochemistry: Conformational analysis of decalin, Elements of symmetry, chirality, molecules with more than one chiral center, methods of resolution , optical purity , enantiotopic and diasterotopic 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. Stereochemistiry 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. Aliphatic nucleophilic substitution: The S_N2, S_N1 mixed S_N1 and S_N2 and SET mechanism. Classical and nonclassical carbocations, phenium ions, norbornyl system.

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 .
Electronic Spectra and Magnetic properties of transition metal complexes: Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra. Spectroscopic method of assignment of absolute configuration of metal chelates and their stereochemical information. Anomalous magnetic moments, magnetic exchange coupling and spin cross over.

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.

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, 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- Blodget 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

ACC32131 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.

ACC32132 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)

ACC32133 Chemistry Practical III (0 0 3)

Adsorption: study of 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 hygrogen 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.

II 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.

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.
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, $\propto$, β decay, γ emission, artificial radioactivity. Nuclear Reactions: Elastic, inelastic, Photonuclear, radiactive 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.

AMC32102 Object Oriented Programming (3 0 0)
OOPs: Basic concepts of OOPs, C++ preliminaries, Data types, Arrays, Functions, Classes and objects, Constructors and destructors, Function overloading, Operator overloading and type conversions, Inheritance, Pointers, Polymorphisms, Console oriented I/O operations, File management, Templates, Exception handling.

Practical

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- $[Co\ (en)_2Cl_2]^+$
Preparation of Cr (III) complexes: $[Cr(H_2O)_6]\ NO_3.3H_2O$, $[Cr(H_2O)_4Cl_2]Cl.2H_2O$, $[Cr(en)_3]Cl_3$, $Cr(acac)_3$.
Preparation of triphenylphosphine Ph_3P and its transition metal complexes
Preparation of cis and trans complexes of Cu with glycine

ACC32235 Chemistry Practical V (0 0 3)
.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. KCI) 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 head of solution.

AMC32202 Object Oriented Programming Lab (0 0 2)

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 uniary 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

ACC32239 Computer applications in Chemistry Lab (0 0 3)

Computer programs on Gauss elimination, Jacobi and Gauss-Seidel methods.
Computer simulation of Potentiometric and Conductometric acid base titration curves
Computer program for multicomponent analysis by spectrophotometry

III 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 diffration; types of close packing - hcp and ccp, packing efficiency, radius ratios; structure types -NaCl, ZnS, Na_2O, $CdCl_2$, wurtzite, nickel arsenide, CsCl, CdI_2, rutile and Cs_2O, perovskite ABO_3, K_2NiF_4, 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 Tc 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.

ACC33141 Introduction to Biochemistry (3 0 0)

Metal Storage Transport and Biomineralization: Ferritin, transferring, 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 oxatransferase enzymes-xanthine oxidase. Coenzyme vitamin B_{12}.
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

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 Quadrapole 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, Cu, Pd, Ni, Rh, Pt, Si and B.
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 5 and 6-membered rings, aromatic heterocycles in organic synthesis.
Synthesis of some complex molecues: camphor, cortisone. Molecul;ar recognition, Supramolecular chemistry, Green chemistry, Sharpless Asymmetric epoxidation.

ACE33145 Advanced Electrochemistry (3 0 0)

Electrodics: 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

Practical

ACC33236 Chemistry Practical VI (0 0 3)

Complete assay of a silicates and ores, using classical and instrumental methods. Characterization of a few polymers using DSC, FTIR and SEM. Characterization of fly ash. Particle size distribution of coal/ash/clay..Characterization of lubricant. Determination of exchange capacity of a few resins.

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.Synthesisofcyclohexylidenecyanoacetates, 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 spectrophometry: Determination of As, Fe, Cr
IR spectrophotometry: Sample preparation, identification of functional groups.

IV 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, ^{1}H, ^{13}C, ^{19}F and ^{31}P, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution. ^{1}H-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 spin systems, simplification of second order spectra. High field NMR, double irradiation, selective decoupling, chemical shift reagents. ^{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, biphenyls, annulenes). 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, molecular ions, fragmentation processes of organic molecules and deduction of structural information.
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.

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 geometrics, classification of fluxional organometallic compounds.
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.