mosaic of ladies finger, quick wilt of pepper, Defense mechanism- systemic acquired resistance and induced systemic resistance, Quarantine., Plant disease controls-chemical, physical and biocontrol agents

04. Chemistry

Unit I
Inorganic Chemistry

Module 1. Periodicity and Chemistry of Main Group Elements

- Periodic properties of elements and periodic trends in physical and chemical properties. Anomalies in periodic properties of the nonmetals and post transition metals. Concepts of resonance and hybridization. VSEPR model. General discussion on main group elements. Noble gas compounds. Classification, Preparation, Properties, Application and Structure of borides, carbides, nitrides, silicates, silicones and, fullerenes. Inter halogen and pseudo-halogen compounds. Boron hydrides and carboranes- Styx numbers and Wade's rule. Borazines, P-N compounds,S-N compounds and molecular sulfides of phosphorus.

Module 2. Chemistry of transition and inner transition elements

- Transition Elements - Electronic configuration, oxidation state and general characteristics. First, second and third rows of transition elements and their important compounds. Isopoly and heteropoly acids of Mo and W. Lanthanides and Actinides - Occurrence, electronic configuration, oxidation state, atomic and ionic radii, ions. Difference between 4*f* and 5*f* orbitals. Separation of Lanthanides and Actinides Lanthanide and Actinide contractions and their consequences. Use of Lanthanide complexes. NMR shift reagents. Magnetic and spectral properties. Applications of Lanthanides, Actinides and their compounds. Trans actinide elements. Super heavy elements.

Module 3. Co-ordination chemistry

- Nomenclature of coordination compounds. Isomerism and stability. HSAB Principle.VB theory, Spectrochemical series and crystal field theory. Splitting of levels in Cubic, Td, Oh, TBP, square pyramidal and Tetragonal ligand fields, MO theory (Tetrahedral and Octahedral complexes with sigma and pi bonding). Reaction mechanism – Dissociative, Associative and Conjugate Base mechanisms. Electron transfer reactions- Inner sphere and outer sphere mechanisms. *Trans* -effect. Jahn- Teller effect and its consequences. Electronic spectra of transition metal complexes, selection rules, Term symbols, Orgel diagram, Racah parameters. Nephelauxetic effect. Charge- transfer spectra. Magnetic properties of transition metal complexes, Spin- only formula, quenching of orbital magnetic moment, Spin orbit coupling. Measurement of magnetic moment. Paramagnetism, diamagnetism, ferromagnetism, ferrimagnetism and antiferromagnetism.

Module 4. Organometallic chemistry

- Types of organometallic compounds, 18 electron rule and Hapticity. Metal carbonyls General properties, nature of bonding ,structure and shapes of metal carbonyls of V, Cr, Mn, Fe, Ru, Co, Rh, Ni, metal alkane and alkene complexes, metal sandwich compounds - ferrocene, dibenzene chromium. Fluxional organometallics. Metal carbenes. Metal clusters as catalysts. Applications of organometallic compounds Hydrogenation, hydroformylation, Wacker's process, Ziegler- Natta catalysis, Monsanto acetic acid process.

Module 5. Bioinorganic chemistry

- Metals and non- metals in biological systems. Metal ion excess and deficiency.Role of alkali- and alkaline earth metal ions in biological systems. Na/K pump. Ca pump. Role of Iron, Copper, Zinc, Manganese,

Cobalt and Molybdenum in biological systems. Iron storage and transport. Haemoglobin, Myoglobin, Hemoerythrin and Haemocyanines- structure and functions. Iron-sulfur proteins, Rubredoxin and Ferredoxins. Cytochromes, SOD's. Photosynthesis, PSI and PSII. Vitamin B12 structure and functions, Nitrogen fixation. Metal ions in medicine and therapy.

Unit II
Organic Chemistry

Module 1. Electron displacement effects and Aromaticity

- Electron displacements - Inductive, Electromeric, Mesomeric and Hyper conjugative effects.
- Resonance. Reactive intermediates, formation and stability of carbocation, carbanion, carbenes, nitrene, benzyne and free radicals . Type of organic reactions - Substitution, Addition, Elimination and Rearrangement reactions. Free radical reactions. Huckel's rule. Homo, hetero and non benzenoid aromatic systems. Aromaticity of annulenes. Cyclic carbocations and carbanions. Antiaromaticity.

Module 2. Reagents and Name Reactions

- Synthetic reagents: Synthetic applications of the following reagents. Grignard reagents, Alkyl lithiums, Gillmann reagent, NBS, Diazomethane, DCC, SeO_2, MCPBA, DDQ, LDA, DiBAL, OsO_4, $NaBH_4$,/$LiBH_4$ and $NaBH_4$/ $AlCl_3$ only) Mannich, Reimer-Tiemann, Reformatsky, Ullmann, Stork enamine,Diels-Alder, Grignard and MPV reactions. Aldol, Cannizzaro, Perkin, Dieckmann, Thorpe and acyloin condensations. Birch, Wolff-Kishner and Clemmensen reductions. Hydroboration and Oppenauer oxidation. Rearrangements - 1,2, shifts 1,3, shifts, Pinacol-Pinacolone, Claisen, Cope, Wagner- Meerwin, Fries, Beckmann and Curtius, Hoffmann and Schmidt rearrangements.

Module 3. Stereochemistry

- Molecular chirality-enantiomers, diastereomers, stereochemical nomenclature, optical activity. Recemisation, Resolution, Conformational analysis of cycloalkanes, Conformational analysis of disubstituted cyclohexane derivatives, stereoselective and stereospecific reactions. Assigning-configuration and conformation – R,S and E,Z nomenclature. Stereochemistry of chiral compounds, dissymmetry, asymmetry, simple and alternating axis of symmetry. Asymmetric synthesis.

Module 4. Photochemistry and Pericyclic Reactions

- Laws of photochemistry, Radiative and non radiative transitions. Fluorescence and quenching. Photosensitisation, Photo-isomerisation and Photosubstitution reactions. Chemiluminescence. Flourescence and Phosphorescence. IC and ISC. Cis-trans isomerization, Paterno-Buchi reaction, Norrish Type I and II reactions, di-pi methane rearrangement, photochemistry of arenes. Selection rules and steriochemistry of electrocyclic reactions, cycloaddition and sigmatropic shifts. Cope and Claisen rearrangements.

Module 5. Natural Products and Biomolecules

- Terpenoids - classification, structure of alpha pinene and Camphor Alkaloids-classification - structure of papavarine and quinine, structure and synthesis of flavones and isoflavons, Lipids - classification and structure. Stereochemistry of steroids-cholesterol. Structure and synthesis of Vitamin A, C, B, K and biotin. Starch, Cellulose, Glycogen. Proteins - Structure, sequence determination in peptides and proteins. Edman degradation. Chemistry of nucleic acid, structure of RNA and DNA.

Unit III
Physical Chemistry

Module 1. Solid, Liquid and Gaseous States

- Crystal systems and lattice types, crystal symmetry. Miller indices-BCC, FCC, HCP,

voids coordination numbers. Molecular, covalent, metallic and hydrogen bonded crystals. Principles of XRD techniques. Determination of lattice type and unit cell dimension of cubic crystals. Electronic structure of solids. Band theory, Electric, Magnetic and Dielectric properties of solids.

- Crystal defects: point, line and plane defects. Crystal structure- Rock salt, Zinc blende, KCl, CsCl, Diamond and Fluorite. Ionic conductors, Diffusion, Super ionic conductors, Phase transitions, Super conductivity. High T_c materials. Magnetic properties of solids. Liquid state - properties, Lennard - Jones theory of melting, Specific heat of liquids. Liquid crystals - types - theories - applications. The distribution of Molecular velocities. Maxwells equation. Average, RMS and Most probable velocities. Influence of temperature on molecular velocities. Mean free path, Effusion. Transport properties: Viscosity, Thermal conductivity and diffusion. Influence of temperature and pressure on transport properties.

Module 2. Thermodynamics

- Laws of Thermodynamics. Thermodynamic properties –Intenal energy, Enthalpy, Entropy, Free energy- their relation and significances. Maxwell relation. Joule-thomson effect. Joule Thomson coefficient. Properties of solutions - Raoult's law, Colligative properties. Thermodynamics of ideal solution. Partial molar quantities. Chemical potentials. Duhem-Margules equation. Excess thermodynamic properties. Fugacity and activity. Chemical Equilibrium - Le Chatelier principle, Homogeneous and Heterogeneous systems. Spontaneity of reactions. Free energy functions.
- Phase Equilibria. Derivation of phase rule. Two component and three component systems. Isothermal evaporation. Irreversible thermodynamics. General theory of non equilibrium processes. Entropy production from heat flow. The phenomenological relations. Onsagar reciprocal relations. Microstates and ensembles, Maxwell - Boltzmann distribution. Quantum Statistics: Bose- Einstein statistics, Fermi - Dirac statistics. Fermi energy, Fermi condensation. Relations between Maxwell - Boltzmann, Bose - Einstein and Fermi-Dirac statistics. The partition functions - translational, vibrational, rotational and electronic. Partition functions and thermodynamics properties. Heat capacity of solids: Dulong-Petits law, Einstein's theory and its modification. Debye's theory.

Module 3. Chemical Kinetics

- Rate laws. Order and molecularity. Determination of order of reactions. Types of reactions - simple & complex, Branching reactions - steady state treatment. Unimolecular reactions Lindemann treatment . Reaction like H_2 -Cl_2, H_2-Br_2 and decomposition of ethane, acetaldehyde Influence of temperature on reaction rate-energy of activation. Theories of reaction rates. Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Reactions in solution: Comparison between reaction in gas phase and in solutions. Factors determining reaction rates in solution-primay and secondary kinetic salt effects. Influence of solvent on reaction rate. Hammet equation. Kinetics of fast reactions. Flash photolysis, flow techniques and relaxation methods.

Module 4. Electrochemistry

- Ions in solution, ionic equilibrium and Electrolysis. Deviation from ideal behaviour, ionic activity ion - solvent interaction. Born equation. Ion - Ion interaction. Activity coefficient and its determination. Debye Huckel limiting law. Debye - Huckel treatment. Onsager equation. Conductance of high frequencies and high potentials. Types of electrodes. Electrochemical cells. Electrochemical series. Electrolytes. Concentration cell and activity coefficient

determination. Liquid junction potential. Evaluation of thermodynamic properties. Electrokinetic phenomena. Electrolysis, current potential curves. Dissolution, deposition and decomposition potentials. Different types of overpotentials. Hydrogen and Oxygen overvoltage. Theories of overvoltage. Corrosion. Anodic and cathodic protection. Galvanization. Tafel plots. Prevention of corrosion. Theories of Fuel cells. H_2-O_2 fuel cells. Fuel cells for high temperature applications.

Module 5. Surface Chemistry, Colloids and Catalysis

- Types of surfaces. Examination of surfaces using ESCA, Auger, SEM and STM.. Thermodynamics of surfaces. Surface tension. Surfactants and miscelles. Surface film. Surface pressure and Surface potential. Adsorption from solutions. Freundlich, Langmuir and BET adsorption isotherms. Physisorption and Chemisorption. Measurement of surface area.
- The colloidal state: Types of colloids. Stability and zeta potential. Properties of colloids. Kinetic, Optical and Electrokinetic. Electrophoresis, Electroosmosis. Donnan membrane equilibrium and its applicaitons. Catalysis: Homogeneous and Heterogenous catalysis. Acid - base catalysis. Langmuir Heinshelwood mechanism. Specific and general catalysis. Acidity function. Theories of catalysis. Langmuir-Hinshelwood and Mars Van Krevelin bonding of reactants to catalyst surfaces. Catalytic oxidation. Industrial applications. Enzyme Catalysis.

Unit IV
Theoretical Chemistry

Module 1. Quantum Mechanics

- Black body radiation, photoelectric effect, Compton effect and atomic spectra. de Broglie hypothesis, Heisenberg uncertainty principle. Postulates of quantum mechanics. Operators, wave function, Eigenfunction and eigenvalue. Orthogonality, normalization, probability and expectation value. Time dependent Schrodinger equation. Time independent Schrodinger eqation for stationary states. Schrodinger wave equation for a free particle, particle in a one - dimensional box. Particle in a Three - dimensional box - Symmetry and degeneracy. Application of quantum mechanics to simple systems. Simple harmonic oscillator. Rigid rotor. Hydrogen - like atoms, Schrodinger wave equation in spherical polar coordinate. Separation of variables. Atomic orbitals, space quantisation, Pertubation theory and variation principle. Time dependant perturbation theory. Self consistent field method. Term symbols, Slater's rule. Slater orbitals. Hartee-Fock self consistent field method for atoms.

Module 2. Chemical Bonding

- Born- Oppenheimer approximation. MO theory of hydrogen molecule ion. MO treatment of homonuclear diatomic molecules- Li_2, Be_2, C_2, N_2, F_2 and heteronuclear diatomic molecules like LiH, CO, NO, HF. Correlation diagrams. Non crossing rules. Spectroscopic Term symbols for diatomic molecules. VB theory of H_2. Resonance. Hybridization – Methane, Water, Ethylene and Acetylene. Types and shapes of polyatomic molecules, VSEPR theory. Semi empirical MO treatment of planar conjugated molecules. Huckel Molecular Orbital method for ethylene, butadiene and allyl systems. Charge distributions and bond orders from the coefficients of HMO, calculation of free valence, HMO theory of aromatic hydrocarbons; Frost-Huckel circle mnemonic device for cyclic polyenes. Intermolecular forces- ion-dipole, dipole-dipole, ion-induced dipole, dipole-induced dipole and dispersion interactions. Lennard - Jones potential.

Module 3. Molecular Symmetry and Group Theory

- Symmetry elements and symmetry operations. Multiplication of operations. Conditions for a set of elements to form a group. Inversion and Improper rotation operation. Point groups and their determination. Abelian and Cyclic groups. Group multiplication table. Sub groups and classes in a group. Similarity transformation and classification of symmetry operations. Reducible and Irreducible representations. Molecular symmetry and Optical activity. Great Orthogonality theorem and rules derived from it. Setting up of character tables of simple groups such as C_{2v} and C_{3v}. The four areas of the character table. Direct product representations. Application of group theory to chemical bonding and molecular vibrations.

Module 4. Molecular Spectroscopy

- Energy levels in molecules principle and selection rules. Born-Oppenheimer approximation. Microwave spectroscopy. Intensity of spectral lines. Calculation of internuclear distance. Rotational spectrum of polyatomic molecules. Vibrational spectroscopy-Harmonic and anharmonic diatomic molecules. Morse function Determination of force constant. Different branches of spectrum. Vibrational spectra of polyatomic molecules, classification of vibrations. Overtones, combination and Fermi resonance. Finger print and group frequencies. Raman Spectra. Polarisability and classical theory of Raman spectrum. Mutual exclusion principle - complementarity of Raman and IR spectra. Electronic Spectra Frank- Condon principle. Types of electronic transitions. Fortrat diagram. Predissociation.. Effect of conjugation on electronic absorption frequencies. Resonance spectroscopy. NMR spectrum. Nuclear spin. Proton NMR chemical shift Relaxation methods. Spin—Spin coupling. ESR spectrum. The 'g' factor. Fine structure and hyperfine structure. Mossbauer spectroscopy.

Module 5. Applications of Spectroscopic Techniques in Chemistry

- U.V.Electronic transition in enes, enones and arenes. Woodward-Fieser rules. Group frequencies. Identification of functional groups with IR. Mass spectrometry, NMR spectroscopy, ^{1}H NMR and ^{13}C NMR - chemical shifts, spin-spin-interactions, spectral interpretations. Applications of IR, NMR, ESR and Mossbauer spectroscopy in coordination chemistry.

Unit V
Analytical Chemistry

Module 1. Basic principles in Analytical Chemistry

- Evaluation of analytical data. Accuracy and precision, standard deviation, variance-confidence limit –Student 't' test, 'F' test. Errors - classification, distribution, propagation, causes and minimisation. Significant figures and computation rules. Titrimetric methods- general principles - Theory and applications of acid-base, redox and complexometric titrations. Theory of Indicators. Gravimetric methods of analysis. Formation of precipitates. Co-precipitation, Post precipitation and peptization. Homogeneous precipitation. Washing, drying and ignition of precipitates.

Module 2. Separation techniques

- Liquid–Liquid extraction, distribution laws. Successive extraction, Craig method. Chromatographic methods, Theory, classification- Column, TLC, PC, HPLC and GC. Detectors. Ion-exchange chromatography. Size exclusion- and Gel permeation chromatography. Affinity- and chiral columns. Normal- and Ultracentrifugation. Electrophoresis.

Module 3. Optical methods of Analysis

- Fundamental laws of Spectrophotometry, Nephelometry, Turbidimetry, Fluorimetry,

Phosphorimetry and AAS. Spectrophotometric titrations. Atomic Emission spectrometry. Excitation sources (flame, AC, DC, arc, spark, ICP, glue discharge and Laser microprobes). Atomisation techniques in AAS, Hollow cathode lamp. interferences back ground corrections. Atomic fluorescence spectrometry. Photoelectron spectroscopy. Analytical applications.

Module 4. Electroanalytical methods

- Basic theory. Conductometric- and Potentiometric titrations. Measurement of pH. Instrumentation and applications of Electrogravimetry, Coulometry, Polarography, Amperometry, Biamperometry, Cyclic Voltammetry, Chronopotentiometry and Stripping analysis.

Module 5. Thermal- and Radiochemical methods

- Theory and applications of Thermogravimetric analysis (TG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC). Thermometric titrations. Radiometric methods, Measurement of radioactivity. Neutron Activation Analysis, Isotopic dilution techniques, Liquid scintillators. Radiometric titrations.

Unit VI
Selected Topics in Chemistry

Module 1. Green Chemistry

- Principles of Green Chemistry, Tools of Green Chemistry. Green reagents and -solvents, Green reactions. Aldol condensation, Cannizaro reaction, Grignard reactions, Green preparations, Phase transfer catalysts. Microwave organic synthesis. Applications of green chemistry. Biocatalysis.

Module 2. Material Chemistry

- Nanomaterials and Nanocomposites. Structure and synthesis. Properties of nanomaterials.- magnetic, optical, electrical and mechanical properties. Applications of nanomaterial in telecommunication, digital technology, biomedical, biomimetics and drug delivery. Quantum dots. Ceramic and composite materials. Traditional ceramics, structure, types of bonds, phase equilibria in ceramic systems. Classification of composites, fibres and matrices. Ceramic matrix composite materials. Sol-gel process and vapour deposition techniques. Applications of composites.

Module 3. Environmental Chemistry

- Composition of atmosphere. Chemical processes in atmosphere. Photochemical smog. Ozone layer. Green House effect. Acid rain. Chemistry of processes in hydrosphere. Acid-base properties. Alkalinity. BOD and COD. Chemistry of processes in lithosphere. Redox status in soil. Acidity in soil. Ion speciation in soil pollution. Cation exchange capacity and exchange phase compostions. Air, water and soil pollution.

Module 4. Polymers

- Natural and synthetic polymers. Isoprene rule. Types of polymerisation. Change in physical and chemical properties. Molecular weight distribution. Polydispersity Index, Crystallinity and Glass transiton temperature. Synthetic polymers-Polyethylene, Polypropylene, PVC, Teflon, Bakelite, Nylon 6 and Nylon 66. High temperature polymers. Degradation of polymers.

Module 5. Medicinal Chemistry

- Drug discovery and design. Classification of Drugs. Physicochemical factors and biological activities. Receptors and drug action. LD_{50} and IC_{50} values. Synthesis of Paracetamol, Phenobarbital, Diazepam, Sulphamethoxazole, Benzyl pencillin, Chloramphenicol.