

CHEMICAL TECHNOLOGY

Process Calculations and Thermodynamics:

Laws of conservation of mass and energy; use of tie components; recycle, bypass and purge calculations; degree of freedom analysis. First and Second laws of thermodynamics. First law application to close and open systems. Second law and Entropy, Thermodynamic properties of pure substances: equation of state, properties of mixtures: partial molar properties, fugacity, excess properties and activity coefficients; phase equilibria: predicting VLE of systems; chemical reaction equilibria.

Fluid Mechanics and Mechanical Operations:

Fluid statics, Newtonian and non-Newtonian fluids, Bernoulli's equation, Macroscopic friction factors, energy balance, dimensional analysis, shell balances, flow through pipeline systems, flow meters, pumps and compressors, packed and fluidized beds, elementary boundary layer theory, size reduction and size separation; free and hindered settling; centrifuge and cyclones; thickening and classification, filtration, mixing and agitation; conveying of solids.

Heat Transfer:

Conduction, convection and radiation, heat transfer coefficients, steady and unsteady heat conduction, boiling, condensation and evaporation; types of heat exchangers and evaporators and their design.

Mass Transfer: Fick's law, molecular diffusion in fluids, mass transfer coefficients, film, penetration and surface renewal theories; momentum, heat and mass transfer analogies; stage wise and continuous contacting and stage efficiencies; HTU & NTU concepts design and operation of equipment for distillation, absorption, leaching, liquid-liquid extraction, drying, humidification, dehumidification and adsorption.

Chemical Reaction Engineering:

Theories of reaction rates; kinetics of homogeneous reactions, interpretation of kinetic data, single and multiple reactions in ideal reactors, non-ideal reactors; residence time distribution, single parameter model; non-isothermal reactors; kinetics of heterogeneous catalytic reactions; diffusion effects in catalysis.

Instrumentation and Process Control: Measurement of process variables; sensors, transducers and their dynamics, transfer functions and dynamic responses of simple systems, process reaction curve, controller modes (P, PI, and PID); control valves; analysis of closed loop systems including stability, frequency response and controller tuning, cascade, feed forward control.

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CHEMISTRY

Unit-1: Chemistry of non- transition and transition elements: General discussion on the properties of the non-transition elements; Allotropy of Carbon, Graphitic compounds, Carbides, Carboranes, Oxides and Oxy – acids of Phosphorous: Phosphazenes. Electronic structure and Oxidation states of Halogens; Interhalogen Compounds; Pseudo halogens and Pseudo halides; Chemistry of Xenon; Structure and Bonding in Xenon compounds. Co-ordination chemistry of transition metal ions, valence bond theory, Crystal field theory splitting of d-orbitals, Jahn-Teller effect, electronic spectra, Nephelauxetic effect, Zeeman and Stark effect, Spectral and magnetic properties of f-block elements.

Unit-2: Catalysis: Types of Catalytic Reagents; Types of Catalysis; Theory of Homogeneous catalysis; Theory of Heterogeneous catalysis; Kinetics of heterogeneous reactions. Specificity in Enzyme Catalyzed reactions; Michaelis- Menten mechanism; Influence of Concentration and temperature on Enzyme-Catalyzed reactions; Acid-base catalysis.

Unit-3: Chemical Kinetics: Introduction to Kinetics; first order, second order and third order reactions; Fast reactions; Rate constants of fast reactions; their determination. Ionic reactions; Influence of solvent on the rate of reactions; Primary salt effect; Secondary salt effect; Influence of frequency factor; Influence of ionic strength.

Unit-4: Stereochemistry: Classification of isomers into structural and stereo types-Optical Isomerism - Elements of symmetry and chirality - Configuration of optically active molecules - DL and RS notations - Relative and Absolute configurations- Resolution of Racemic mixtures. Absolute asymmetric synthesis - Asymmetric induction - Stereospecific and Regiospecific synthesis - Cram's rule - Optical Isomerism of Nitrogen compounds - Concept of dynamic enantiomerism. Cis-Trans isomerism; E-Z configuration - Interconversion of geometrical isomers and determination of their configuration; Stereo chemistry of oximes and Beckmann rearrangement - Conformational analysis of acyclic systems like ethane and n-butane and cyclic systems like cyclohexane.

Unit-5: UV-Visible and IR Spectroscopy: Introduction; Absorption Laws; Theory of Electronic Spectroscopy; Chromophore concept; Auxochrome; Solvent effect; Instrumentation; Woodward – Fischer rules for calculating absorption maxima in dienes and α,β -unsaturated carbonyl compounds; Steric hindrances and co-planarity; Estimation of ligand-metal ratio in complexes; Applications.

IR Spectroscopy: IR spectrometer, Sampling techniques, Interpretation and applications of IR Spectra.

Unit-6: Elimination and Substitution Reactions: Classification E_1 , E_2 , E_1CB and Pyrolytic mechanism – Orientation in elimination reaction – Hofmann and Zaitsev products.

Substitution Reactions: substitution in benzene; formation of σ and π complexes; Orientation and Reactivity in benzene ring containing one and more than one substituent; Directing effect of substituent already on benzene ring; Effect of electrophile; Effect of leaving group ; Orientation and Reactivity in naphthalene, phenanthrene and Anthracene;

Electrophilic aromatic substitution in activated benzene derivatives; Reimer-Tiemann reaction; Vilsmeier-Haack reaction; Houben-Hoesch reaction; Diazo-Coupling; Hofmann -Martius rearrangement.; Aryl halides; Low reactivity of aryl and vinyl halides; SN^1 , SN^2 and benzyne mechanisms; Reactivity and Orientation in nucleophilic aromatic substitution; Von-Richter rearrangement and Sommelet- Hauser rearrangement.

Unit-7: NMR Spectroscopy: Principles of NMR Spectroscopy; Characteristics of a PMR Spectrum such as number of signals, Chemical shift, Integration, Spin-Spin coupling etc. Ring current effects Aromaticity, Diamagnetic Anisotropic effects. Mechanics of Measurement; Instrumentation for Continuous wave PMR; Nuclear Magnetic Resonance – A closer look; Coupling constants; Karplus Equation; Vicinal, geminal, vinylic and aromatic protons. Protons bound to heteroatoms; Protons bound to Oxygen – Effect of hydrogen bonding & chemical exchange; Spectrum of ethanol; Protons bound to Nitrogen; Effect of nuclear quadrupole moment; D₂O exchange process; Hindered rotation; Spectrum of Dimethyl formamide. Simplification of PMR spectrum; Higher Resolution NMR; Double Resonance technique; Lanthanide shift reagents. ¹³C NMR Spectroscopy; CW & FT methods; Proton Noise Decoupled and Off-Resonance Spectra; 2D – NMR spectroscopy; NOESY & COESY Techniques.

Unit-8: Mass Spectroscopy and ESR Spectroscopy: Basic principles; Instrumentation – The electron –impact mass spectrometer; GC-MS and Double Focussing instruments; Types of ions in the mass spectrometer – Meta-stable peaks – Mass spectral fragmentation patterns of some select class of organic compounds such as hydrocarbons, alcohols, acids etc. - Mc Lafferty rearrangement:
Instrumentation of ESR, Quantitative analysis; Study of free radicals; Structure determination; Analytical applications.

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