GATE Syllabus

Chemistry

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CHEMISTRY

Subject Code: CY

Course Structure

Sections/Units	Topics
Section A	**Physical Chemistry**
Unit 1	Structure
Unit 2	Equilibrium
Unit 3	Kinetics
Unit 4	Surfaces and Interfaces
Section B	**Inorganic Chemistry**
Unit 1	Main Group Elements
Unit 2	Transition Elements
Unit 3	Lanthanides and Actinides
Unit 4	Organometallics
Unit 5	Radioactivity
Unit 6	Bioinorganic Chemistry
Unit 7	Solids
Unit 8	Instrumental Methods of Analysis
Section C	**Organic Chemistry**
Unit 1	Stereochemistry
Unit 2	Reaction Mechanisms
Unit 3	Organic Synthesis
Unit 4	Pericyclic Reactions and Photochemistry

Unit 5	Heterocyclic Compounds
Unit 6	Biomolecules
Unit 7	Spectroscopy

Course Syllabus

Section A: Physical Chemistry

Unit 1: Structure

- Postulates of quantum mechanics
- Time dependent and time independent Schrödinger equations
- Born interpretation
- Particle in a box
- Harmonic oscillator
- Rigid rotor
- Hydrogen atom: atomic orbitals
- Multi-electron atoms: orbital approximation
- Variation and first order perturbation techniques
- Chemical bonding: Valence bond theory and LCAO-MO theory
- Hybrid orbitals
- Applications of LCAO-MOT to H_2+, H_2 and other homonuclear diatomic molecules, heteronuclear diatomic molecules like HF, CO, NO, and to simple delocalized π– electron systems
- Hückel approximation and its application to annular π – electron systems
- Symmetry elements and operations
- Point groups and character tables
- Origin of selection rules for rotational, vibrational, electronic and Raman spectroscopy of diatomic and polyatomic molecules
- Einstein coefficients
- Relationship of transition moment integral with molar extinction coefficient and oscillator strength
- Basic principles of nuclear magnetic resonance: nuclear g factor, chemical shift, nuclear coupling

Unit 2: Equilibrium

- Laws of thermodynamics
- Standard states

- Thermochemistry
- Thermodynamic functions and their relationships:
  - Gibbs-Helmholtz and Maxwell relations
  - Van't Hoff equation
- Criteria of spontaneity and equilibrium
- Absolute entropy
- Partial molar quantities
- Thermodynamics of mixing
- Chemical potential
- Fugacity, activity and activity coefficients
- Chemical equilibria
- Dependence of equilibrium constant on temperature and pressure
- Non-ideal solutions
- Ionic mobility and conductivity
- Debye-Hückel limiting law
- Debye-Hückel-Onsager equation
- Standard electrode potentials and electrochemical cells
- Potentiometric and conductometric titrations
- Phase rule
- Clausius Clapeyron equation
- Phase diagram of one component systems: CO_2, H_2O, S
- Two component systems:
  - Liquid-vapour system
  - Liquid-liquid system
  - Solid-liquid systems
- Fractional distillation
- Azeotropes and eutectics
- Statistical thermodynamics:
  - Microcanonical and canonical ensembles
  - Boltzmann distribution
  - Partition functions
  - Thermodynamic properties

Unit 3: Kinetics

- Transition state theory:
  - Eyring equation
  - Thermodynamic aspects
- Potential energy surfaces and classical trajectories
- Elementary, parallel, opposing and consecutive reactions
- Steady state approximation
- Mechanisms of complex reactions

- Unimolecular reactions
- Kinetics of polymerization and enzyme catalysis
- Fast reaction kinetics: relaxation and flow methods
- Kinetics of photochemical and photophysical processes

Unit 4: Surfaces and Interfaces

- Physisorption and chemisorption
- Langmuir, Freundlich and BET isotherms
- Surface catalysis: Langmuir-Hinshelwood mechanism
- Surface tension, viscosity
- Self-assembly
- Physical chemistry of colloids, micelles and macromolecules

Section B: Inorganic Chemistry

Unit 1: Main Group Elements

- Hydrides, halides, oxides, oxoacids, nitrides, sulfides – shapes and reactivity
- Structure and bonding of boranes, carboranes, silicones, silicates, boron nitride, borazines and phosphazenes
- Allotropes of carbon
- Chemistry of noble gases, pseudohalogens, and interhalogen compounds
- Acid-base concepts

Unit 2: Transition Elements

- Coordination chemistry:
  - structure and isomerism
  - Theories of bonding (VBT, CFT, and MOT)
- Energy level diagrams in various crystal fields, CFSE, applications of CFT, Jahn-Teller distortion
- Electronic spectra of transition metal complexes:
  - Spectroscopic term symbols
  - Selection rules
  - Orgel diagrams
  - Charge-transfer spectra
- Magnetic properties of transition metal complexes
- Reaction mechanisms:
  - Kinetic and thermodynamic stability
  - Substitution and redox reactions

Unit 3: Lanthanides and Actinides

- Recovery
- Periodic properties
- Spectra properties
- Magnetic properties

Unit 4: Organometallics

- 18-Electron rule
  - metal-alkyl
  - metal-carbonyl
  - metal-olefin and metalcarbene complexes
  - metallocenes
- Fluxionality in organometallic complexes
- Types of organometallic reactions
- Homogeneous catalysis:
  - Hydrogenation
  - Hydroformylation
  - Acetic acid synthesis
  - Metathesis and olefin oxidation
- Heterogeneous catalysis:
  - Fischer-Tropsch reaction
  - Ziegler-Natta polymerization

Unit 5: Radioactivity

- Decay processes
- Half-life of radioactive elements
- Fission and fusion processes

Unit 6: Bioinorganic Chemistry

- Ion (Na^+ and K^+) transport
- Oxygen binding
- Transport and utilization
- Electron transfer reactions
- Nitrogen fixation
- Metalloenzymes containing:
  - Magnesium
  - Molybdenum

- Iron
- Cobalt
- Copper
- Zinc

Unit 7: Solids

- Crystal systems and lattices
- Miller planes
- Crystal packing
- Crystal defects
- Bragg's law
- Ionic crystals
- Structures of AX, AX2, ABX3 type compounds
- Spinels
- Band theory
- Metals
- Semiconductors

Unit 8: Instrumental Methods of Analysis

- UV-visible spectrophotometry
- NMR and ESR spectroscopy
- Mass spectrometry
- Chromatography including GC and HPLC
- Electroanalytical methods:
  - Polarography
  - Cyclic voltammetry
  - Ion-selective electrodes
- Thermoanalytical methods

Section C: Organic Chemistry

Unit 1: Stereochemistry

- Chirality of organic molecules with or without chiral centres and determination of their absolute configurations
- Relative stereochemistry in compounds having more than one stereogenic centre
- Homotopic, enantiotopic and diastereotopic atoms, groups and faces
- Stereoselective and stereospecific synthesis

- Conformational analysis of acyclic and cyclic compounds
- Geometrical isomerism
- Configurational and conformational effects, and neighbouring group participation on reactivity and selectivity/specificity

Unit 2: Reaction Mechanisms

- Basic mechanistic concepts:
  - Kinetic versus thermodynamic control
  - Hammond's postulate and Curtin-Hammett principle
- Methods of determining reaction mechanisms through identification of products, intermediates and isotopic labeling
- Nucleophilic and electrophilic substitution reactions (both aromatic and aliphatic)
- Addition reactions to carbon-carbon and carbon-heteroatom (N, O) multiple bonds
- Elimination reactions
- Reactive intermediates:
  - Carbocations
  - Carbanions
  - Carbenes
  - Nitrenes
  - Arynes
  - Free radicals
- Molecular rearrangements involving electron deficient atoms

Unit 3: Organic Synthesis

- Synthesis, reactions, mechanisms and selectivity involving the following classes of compounds:
  - Alkenes
  - Alkynes
  - Arenes
  - Alcohols
  - Phenols
  - Aldehydes
  - Ketones
  - Carboxylic acids
  - Esters
  - Nitriles
  - Halides
  - Nitro compounds

    - Amines and amides
- Uses of Mg, Li, Cu, B, Zn and Si based reagents in organic synthesis
- Carbon-carbon bond formation through coupling reactions - Heck, Suzuki, Stille and Sonogoshira
- Concepts of multistep synthesis:
    - Retrosynthetic analysis
    - Strategic disconnections
    - Synthons and synthetic equivalents
- Umpolung reactivity – formyl and acyl anion equivalents
- Selectivity in organic synthesis – chemo-, regio- and stereoselectivity
- Protection and deprotection of functional groups
- Concepts of asymmetric synthesis – resolution (including enzymatic), desymmetrization and use of chiral auxiliaries
- Carbon-carbon bond forming reactions through enolates (including boron enolates), enamines and silyl enol ethers.
- Michael addition reaction
- Stereoselective addition to C=O groups (Cram and Felkin-Anh models)

Unit 4: Pericyclic Reactions and Photochemistry

- Electrocyclic, cycloaddition and sigmatropic reactions
- Orbital correlations - FMO and PMO treatments
- Photochemistry of alkenes, arenes and carbonyl compounds
- Photooxidation and photoreduction
- Di-π-methane rearrangement, Barton reaction

Unit 5: Heterocyclic Compounds

- Structure
- Preparation
- Properties and reactions of furan
- Pyrrole
- Thiophene
- Pyridine
- Indole
- Quinolone
- Isoquinoline

Unit 6: Biomolecules

- Structure
- Properties and reactions of mono- and di-saccharides
- Physicochemical properties of amino acids
- Chemical synthesis of peptides
- Structural features of proteins
- Nucleic acids
- Steroids
- Terpenoids
- Carotenoids
- Alkaloids

Unit 7: Spectroscopy

- Applications of UV-visible, IR, NMR and Mass spectrometry in the structural determination of organic molecules