

## **PHYSICAL SCIENCES**

### **PART 'A' CORE**

#### **I. Mathematical Methods of Physics**

Dimensional analysis. Vector algebra and vector calculus. Linear algebra, matrices, Cayley-Hamilton Theorem. Eigenvalues and eigenvectors. Linear ordinary differential equations of first & second order, Special functions (Hermite, Bessel, Laguerre and Legendre functions). Fourier series, Fourier and Laplace transforms. Elements of complex analysis, analytic functions; Taylor & Laurent series; poles, residues and evaluation of integrals. Elementary probability theory, random variables, binomial, Poisson and normal distributions. Central limit theorem.

#### **II. Classical Mechanics**

Newton's laws. Dynamical systems, Phase space dynamics, stability analysis. Central force motions. Two body Collisions - scattering in laboratory and Centre of mass frames. Rigid body dynamics- moment of inertia tensor. Non-inertial frames and pseudoforces. Variational principle. Generalized coordinates. Lagrangian and Hamiltonian formalism and equations of motion. Conservation laws and cyclic coordinates. Periodic motion: small oscillations, normal modes. Special theory of relativity- Lorentz transformations, relativistic kinematics and mass-energy equivalence.

#### **III. Electromagnetic Theory**

Electrostatics: Gauss's law and its applications, Laplace and Poisson equations, boundary value problems. Magnetostatics: Biot-Savart law, Ampere's theorem. Electromagnetic induction. Maxwell's equations in free space and linear isotropic media; boundary conditions on the fields at interfaces. Scalar and vector potentials, gauge invariance. Electromagnetic waves in free space. Dielectrics and conductors. Reflection and refraction, polarization, Fresnel's law, interference, coherence, and diffraction. Dynamics of charged particles in static and uniform electromagnetic fields.

#### **IV. Quantum Mechanics**

Wave-particle duality. Schrödinger equation (time-dependent and time-independent). Eigenvalue problems (particle in a box, harmonic oscillator, etc.). Tunnelling through a barrier. Wave-function in coordinate and momentum representations. Commutators and Heisenberg uncertainty principle. Dirac notation for state vectors. Motion in a central potential: orbital angular momentum, angular momentum algebra, spin, addition of angular momenta; Hydrogen atom. Stern-Gerlach experiment. Time independent perturbation theory and applications. Variational method. Time dependent perturbation theory and Fermi's golden rule, selection rules. Identical particles, Pauli exclusion principle, spin-statistics connection.

#### **V. Thermodynamic and Statistical Physics**

Laws of thermodynamics and their consequences. Thermodynamic potentials, Maxwell relations, chemical potential, phase equilibria. Phase space, micro- and macro-states. Micro-canonical, canonical and grandcanonical ensembles and partition functions. Free energy and its connection with thermodynamic quantities. Classical and quantum statistics. Ideal Bose and Fermi gases. Principle of detailed balance. Blackbody radiation and Planck's distribution law.

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**VI. Electronics and Experimental Methods**

Semiconductor devices (diodes, junctions, transistors, field effect devices, homo- and hetero-junction devices), device structure, device characteristics, frequency dependence and applications. Opto-electronic devices (solar cells, photo-detectors, LEDs). Operational amplifiers and their applications. Digital techniques and applications (registers, counters, comparators and similar circuits). A/D and D/A converters. Microprocessor and microcontroller basics.

Data interpretation and analysis. Precision and accuracy. Error analysis, propagation of errors. Least squares fitting,

**PART 'B' ADVANCED**

**I. Mathematical Methods of Physics**

Green's function. Partial differential equations (Laplace, wave and heat equations in two and three dimensions). Elements of computational techniques: root of functions, interpolation, extrapolation, integration by trapezoid and Simpson's rule, Solution of first order differential equation using Runge Kutta method. Finite difference methods. Tensors. Introductory group theory: SU(2), O(3).

**II. Classical Mechanics**

Dynamical systems, Phase space dynamics, stability analysis. Poisson brackets and canonical transformations. Symmetry, invariance and Noether's theorem. Hamilton-Jacobi theory.

**III. Electromagnetic Theory**

Dispersion relations in plasma. Lorentz invariance of Maxwell's equation. Transmission lines and wave guides. Radiation- from moving charges and dipoles and retarded potentials.

**IV. Quantum Mechanics**

Spin-orbit coupling, fine structure. WKB approximation. Elementary theory of scattering: phase shifts, partial waves, Born approximation. Relativistic quantum mechanics: Klein-Gordon and Dirac equations. Semi-classical theory of radiation.

**V. Thermodynamic and Statistical Physics**

First- and second-order phase transitions. Diamagnetism, paramagnetism, and ferromagnetism. Ising model. Bose-Einstein condensation. Diffusion equation. Random walk and Brownian motion. Introduction to nonequilibrium processes.

**VI. Electronics and Experimental Methods**

Linear and nonlinear curve fitting, chi-square test. Transducers (temperature, pressure/vacuum, magnetic fields, vibration, optical, and particle detectors). Measurement and control. Signal conditioning and recovery. Impedance matching, amplification (Op-amp based, instrumentation amp, feedback), filtering and noise reduction, shielding and grounding. Fourier transforms, lock-in detector, box-car integrator, modulation techniques. High frequency devices (including generators and detectors).

**VII. Atomic & Molecular Physics**

Quantum states of an electron in an atom. Electron spin. Spectrum of helium and alkali atom. Relativistic corrections for energy levels of hydrogen atom, hyperfine structure and isotopic shift, width of spectrum lines,

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LS & JJ couplings. Zeeman, Paschen-Bach & Stark effects. Electron spin resonance. Nuclear magnetic resonance, chemical shift. Frank-Condon principle. Born-Oppenheimer approximation. Electronic, rotational, vibrational and Raman spectra of diatomic molecules, selection rules. Lasers: spontaneous and stimulated emission, Einstein A & B coefficients. Optical pumping, population inversion, rate equation. Modes of resonators and coherence length.

**VIII. Condensed Matter Physics**

Bravais lattices. Reciprocal lattice. Diffraction and the structure factor. Bonding of solids. Elastic properties, phonons, lattice specific heat. Free electron theory and electronic specific heat. Response and relaxation phenomena. Drude model of electrical and thermal conductivity. Hall effect and thermoelectric power. Electron motion in a periodic potential, band theory of solids: metals, insulators and semiconductors. Superconductivity: type-I and type-II superconductors. Josephson junctions. Superfluidity. Defects and dislocations. Ordered phases of matter: translational and orientational order, kinds of liquid crystalline order. Quasi crystals.

**IX. Nuclear and Particle Physics**

Basic nuclear properties: size, shape and charge distribution, spin and parity. Binding energy, semiempirical mass formula, liquid drop model. Nature of the nuclear force, form of nucleon-nucleon potential, chargeindependence and charge-symmetry of nuclear forces. Deuteron problem. Evidence of shell structure, singleparticle shell model, its validity and limitations. Rotational spectra. Elementary ideas of alpha, beta and gamma decays and their selection rules. Fission and fusion. Nuclear reactions, reaction mechanism, compound nuclei and direct reactions.

Classification of fundamental forces. Elementary particles and their quantum numbers (charge, spin, parity, isospin, strangeness, etc.). Gellmann-Nishijima formula. Quark model, baryons and mesons. C, P, and T invariance. Application of symmetry arguments to particle reactions. Parity non-conservation in weak interaction. Relativistic kinematics.

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## CHEMICAL SCIENCES

### Inorganic Chemistry

1. Chemical periodicity
2. Structure and bonding in homo- and heteronuclear molecules, including shapes of molecules (VSEPR Theory).
3. Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents.
4. Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.
5. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms.
6. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.
7. Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis.
8. Cages and metal clusters.
9. Analytical chemistry- separation, spectroscopic, electro- and thermoanalytical methods.
10. Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine.
11. Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.
12. Nuclear chemistry: nuclear reactions, fission and fusion, radio-analytical techniques and activation analysis.

### **Physical Chemistry:**

1. Basic principles of quantum mechanics: Postulates; operator algebra; exactly- solvable systems: particle in a box, harmonic oscillator and the hydrogen atom, including shapes of atomic orbitals; orbital and spin angular momenta; tunneling.
2. Approximate methods of quantum mechanics: Variational principle; perturbation theory up to second order in energy; applications.
3. Atomic structure and spectroscopy; term symbols; many-electron systems and antisymmetry principle.
4. Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated  $\pi$  electron systems.
5. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.
6. Molecular spectroscopy: Rotational and vibrational spectra of diatomic molecules; electronic spectra; IR and Raman activities – selection rules; basic principles of magnetic resonance.

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7. Chemical thermodynamics: Laws, state and path functions and their applications; thermodynamic description of various types of processes; Maxwell's relations; spontaneity and equilibria; temperature and pressure dependence of thermodynamic quantities; Le Chatelier principle; elementary description of phase transitions; phase equilibria and phase rule; thermodynamics of ideal and non-ideal gases, and solutions.
8. Statistical thermodynamics: Boltzmann distribution; kinetic theory of gases; partition functions and their relation to thermodynamic quantities – calculations for model systems.
9. Electrochemistry: Nernst equation, redox systems, electrochemical cells; DebyeHuckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
10. Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.
11. Colloids and surfaces: Stability and properties of colloids; isotherms and surface area; heterogeneous catalysis.
12. Solid state: Crystal structures; Bragg's law and applications; band structure of solids.
13. Polymer chemistry: Molar masses; kinetics of polymerization.
14. Data analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

**Organic Chemistry**

1. IUPAC nomenclature of organic molecules including regio- and stereoisomers.
2. Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction.
3. Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.
4. Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes.
5. Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.
6. Common named reactions and rearrangements – applications in organic synthesis.

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7. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.
8. Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
9. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.
10. Pericyclic reactions – electrocycloisatation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.
11. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).
12. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids.
13. Structure determination of organic compounds by IR, UV-Vis,  $^1\text{H}$  &  $^{13}\text{C}$  NMR and Mass spectroscopic techniques.

**Interdisciplinary topics**

1. Chemistry in nanoscience and technology.
  2. Catalysis and green chemistry.
  3. Medicinal chemistry.
  4. Supramolecular chemistry.
  5. Environmental chemistry.
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## MATHEMATICAL SCIENCES

### UNIT – 1

**Analysis:** Elementary set theory, finite, countable and uncountable sets, Real number system as a complete ordered field, Archimedean property, supremum, infimum.

Sequences and series, convergence, limsup, liminf.

Bolzano Weierstrass theorem, Heine Borel theorem.

Continuity, uniform continuity, differentiability, mean value theorem.

Sequences and series of functions, uniform convergence.

Riemann sums and Riemann integral, Improper Integrals.

Monotonic functions, types of discontinuity, functions of bounded variation, Lebesgue measure, Lebesgue integral.

Functions of several variables, directional derivative, partial derivative, derivative as a linear transformation, inverse and implicit function theorems.

Metric spaces, compactness, connectedness. Normed linear Spaces. Spaces of continuous functions as examples.

**Linear Algebra:** Vector spaces, subspaces, linear dependence, basis, dimension, algebra of linear transformations. Algebra of matrices, rank and determinant of matrices, linear equations.

Eigenvalues and eigenvectors, Cayley-Hamilton theorem.

Matrix representation of linear transformations. Change of basis, canonical forms, diagonal forms, triangular forms, Jordan forms.

Inner product spaces, orthonormal basis.

Quadratic forms, reduction and classification of quadratic forms

### UNIT – 2

**Complex Analysis:** Algebra of complex numbers, the complex plane, polynomials, power series, transcendental functions such as exponential, trigonometric and hyperbolic functions. Analytic functions, Cauchy-Riemann equations.

Contour integral, Cauchy's theorem, Cauchy's integral formula, Liouville's theorem, Maximum modulus principle, Schwarz lemma, Open mapping theorem.

Taylor series, Laurent series, calculus of residues.

Conformal mappings, Mobius transformations.

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**Algebra:** Permutations, combinations, pigeon-hole principle, inclusion-exclusion principle, derangements.

Fundamental theorem of arithmetic, divisibility in  $Z$ , congruences, Chinese Remainder Theorem, Euler's  $\phi$ -function, primitive roots.

Groups, subgroups, normal subgroups, quotient groups, homomorphisms, cyclic groups, permutation groups, Cayley's theorem, class equations, Sylow theorems.

Rings, ideals, prime and maximal ideals, quotient rings, unique factorization domain, principal ideal domain, Euclidean domain.

Polynomial rings and irreducibility criteria.

Fields, finite fields, field extensions, Galois Theory.

**Topology:** basis, dense sets, subspace and product topology, separation axioms, connectedness and compactness.

**UNIT – 3**

**Ordinary Differential Equations (ODEs):**

Existence and uniqueness of solutions of initial value problems for first order ordinary differential equations, singular solutions of first order ODEs, system of first order ODEs.

General theory of homogenous and non-homogeneous linear ODEs, variation of parameters,

Sturm-Liouville boundary value problem, Green's function.

**Partial Differential Equations (PDEs):**

Lagrange and Charpit methods for solving first order PDEs, Cauchy problem for first order PDEs.

Classification of second order PDEs, General solution of higher order PDEs with constant coefficients, Method of separation of variables for Laplace, Heat and Wave equations.

**Numerical Analysis :**

Numerical solutions of algebraic equations, Method of iteration and Newton-Raphson method, Rate of convergence, Solution of systems of linear algebraic equations using Gauss elimination and Gauss-Seidel methods, Finite differences, Lagrange, Hermite and spline interpolation, Numerical differentiation and integration, Numerical solutions of ODEs using Picard, Euler, modified Euler and Runge-Kutta methods.

**Calculus of Variations:**

Variation of a functional, Euler-Lagrange equation, Necessary and sufficient conditions for extrema. Variational methods for boundary value problems in ordinary and partial differential equations.

**Linear Integral Equations:**

Linear integral equation of the first and second kind of Fredholm and Volterra type, Solutions with separable kernels. Characteristic numbers and eigenfunctions, resolvent kernel.

**Classical Mechanics:**

Generalized coordinates, Lagrange's equations, Hamilton's canonical equations, Hamilton's principle and principle of least action, Two-dimensional motion of rigid bodies, Euler's dynamical equations for the motion of a rigid body about an axis, theory of small oscillations.

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**UNIT – 4**

Descriptive statistics, exploratory data analysis

Sample space, discrete probability, independent events, Bayes theorem. Random variables and distribution functions (univariate and multivariate); expectation and moments. Independent random variables, marginal and conditional distributions. Characteristic functions. Probability inequalities (Tchebyshef, Markov, Jensen). Modes of convergence, weak and strong laws of large numbers, Central Limit theorems (i.i.d. case).

Markov chains with finite and countable state space, classification of states, limiting behaviour of n-step transition probabilities, stationary distribution, Poisson and birth-and-death processes.

Standard discrete and continuous univariate distributions. sampling distributions, standard errors and asymptotic distributions, distribution of order statistics and range.

Methods of estimation, properties of estimators, confidence intervals. Tests of hypotheses: most powerful and uniformly most powerful tests, likelihood ratio tests. Analysis of discrete data and chi-square test of goodness of fit. Large sample tests.

Simple nonparametric tests for one and two sample problems, rank correlation and test for independence. Elementary Bayesian inference.

Gauss-Markov models, estimability of parameters, best linear unbiased estimators, confidence intervals, tests for linear hypotheses. Analysis of variance and covariance. Fixed, random and mixed effects models. Simple and multiple linear regression. Elementary regression diagnostics. Logistic regression.

Multivariate normal distribution, Wishart distribution and their properties. Distribution of quadratic forms. Inference for parameters, partial and multiple correlation coefficients and related tests. Data reduction techniques: Principle component analysis, Discriminant analysis, Cluster analysis, Canonical correlation.

Simple random sampling, stratified sampling and systematic sampling. Probability proportional to size sampling. Ratio and regression methods.

Completely randomized designs, randomized block designs and Latin-square designs. Connectedness and orthogonality of block designs, BIBD.  $2_k$  factorial experiments: confounding and construction.

Hazard function and failure rates, censoring and life testing, series and parallel systems.

Linear programming problem, simplex methods, duality. Elementary queuing and inventory models.

Steady-state solutions of Markovian queuing models: M/M/1, M/M/1 with limited waiting space, M/M/C, M/M/C with limited waiting space, M/G/1.

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**LIFE SCIENCES**

**Sequence analysis**

Scoring matrices: Detailed method of derivation of the PAM and BLOSUM matrices, Pairwise sequence alignments: Needleman and Wunsch, Smith and Waterman algorithms and their implementation. Multiple sequence alignments (MSA). Use of HMM-based Algorithm for MSA. Sequence patterns and profiles: Repeats-Tandem and Interspersed repeats, repeat finding, Motifs, consensus, position weight matrices. Algorithms for derivation of and searching sequence patterns: MEME, PHI-BLAST, SCanProsite.

Algorithms for generation of sequence profiles: Profile Analysis method of Gribskov, HMMer, PSIBLAST. Protein and nucleic acid properties: e.g. Proteomics tools at the ExPASy server and EMBOSS, Taxonomy and phylogeny: Phylogenetic analysis algorithms such as maximum Parsimony, UPGMA, Transformed Distance, NeighborsRelation, Neighbor-Joining, Probabilistic models and associated algorithms such as Probabilistic models of evolution and maximum likelihood algorithm, Bayesian inference algorithm, Bootstrapping methods, use of tools such as PHYLIP, MEGA, PAUP, Analysis of regulatory RNA's: Databases and tools.

**Genomics**

Gene networks: basic concepts, computational model such as Lambda receptor and lac operon Prediction of genes, promoters, splice sites, regulatory regions: basic principles, application of methods to prokaryotic and eukaryotic genomes and interpretation of results. Next Generation sequencing & assembly: Elements of big data analysis, NGS Platforms based on pyrosequencing, sequencing by synthesis; Genome assembly algorithms, De-novo assembly algorithms. Application of sequence based and structure-based approaches to assignment of gene functions– e.g. sequence comparison, structure analysis (especially active sites, binding sites) and comparison, pattern identification, etc. Use of various derived databases in function assignment, use of SNPs for identification of genetic traits, Gene/Protein function prediction using Machine learning tools: supervised/unsupervised learning, Neural network, SVM etc.

**Modeling biological systems**

Systems biology – Topology of biological networks: Random vs Scale-Free networks. Use of computers in simulation of cellular subsystems: Simulation and analysis of biochemical networks and their dynamics using ODEs and stochastic algorithm, Flux Balance Analysis (FBA), Boolean network simulations.

**Structural Biology**

Experimental methods for Biomolecular structure determination: X-ray and NMR Identification/assignment of secondary structural elements from the knowledge of 3-D structure of macromolecule using DSSP and STRIDE methods

Prediction of secondary structure: PHD and PSI-PRED methods, Tertiary Structure prediction: Fundamentals of the methods for 3D structure prediction (sequence similarity/identity of target proteins of known structure, fundamental principles of protein folding etc.) Homology Modeling, fold recognition, threading approaches, and ab -initio structure prediction methods. **Molecular modeling and simulations**

Macro-molecular force fields, salvation, long-range forces, Geometry optimization algorithms: Steepest descent, conjugate gradient, Various simulation techniques: Molecular mechanics, conformational searches, Molecular Dynamics, Monte Carlo, genetic algorithm approaches, Rigid and Semi-Flexible Molecular Docking.

**Drug design**

Structure-based drug design: Identification and Analysis of Binding sites and virtual screening, Ligand based drug design: Structure Activity Relationship – QSARs and QSPRs, QSAR Methodology, Pharmacophore mapping, In silico prediction ADMET properties for Drug Molecules.

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