CHEMISTRY CURRICULUM

SEMESTER – I

Chemistry-I: Physical principles (2:1)

Atomic structure and electronic configuration, Bohr H-atom, Schrödinger Equation, H-atom and atomic orbitals, shapes and spin, many electron atoms etc. Molecules: Octet rule and Lewis dot structures, covalent, coordinate and ionic bonding, valance bond theory, hybridization and resonance; H_2^+ and H_2 molecules and MO, homonuclear and heteronuclear diatomics, potential energy curves; Molecular orbital theory; Atomic and molecular spectroscopy. Gas laws, mean free path, viscosity, Maxwell-Boltzmann distribution of velocity, real gases, van der Waals equation. Laws of thermodynamics, molecular basis of entropy and free energy. Solutions, Raolt's law, Henry's law and colligative properties. Enthalpy of reaction, lattice energies and Born-Haber cycle, ionic equilibrium, Arrhenius law and ionic conductivity. Basic electrochemistry, Nernst Equation and electrochemical cells. Acid and bases, buffers, etc. Rate processes, order, molecularity, differential and integral rate equations, experimental methods for order and rate measurements, half-life, steady-state approximation, Arrhenius equation and collision theory and catalysis.

SEMESTER – II

Chemistry-II: Structure and reactivity (2:1)

Chemical bonding: VBT, resonance, hybridization, VSEPR and Molecular Structure; Molecular orbital theory: polyatomic molecules - Walsh diagram; Main group chemistry: periodic properties, chemistry of the elements of the groups, inter-halogen compounds, noble gases, Acid - base concepts. Symmetry in Molecules, chirality representation of organic structures, isomerism in organic compounds, stereoisomerism, R,S-nomenclature, D,L-designations, optical activity and its measurement, optical purity, enantiomeric excess, topicity and pro-stereoisomerism, racemisation and resolution, conformations of acyclic and cyclic systems. Reactive intermediates: radicals, carbocations, carbanions and their reactions. Types of reactions: Nucleophilic substitution, Elimination reactions, Addition of C=C and C=O: introduction of Hammond's postulate.

SEMESTER – III

Chemistry-III: Materials, Biology and Environment (2:1)

Chemistry of materials: Ordered and disordered solids, close packing in inorganic solids, covalent network solids and molecular solids; Molecular self-assembly and supramolecular systems; Surfactants and colloids. Polymers, Liquid crystals and Non-linear optical materials; Porous solids: ion-exchange, sorbents and catalysis; Nanomaterials. Chemistry of the environment: Atmospheric chemistry, Greenhouse effect, smog and ozone depletion.Chemistry of life process: Amino acids, Peptides and Proteins; Enzymes; Nucleic Acids, Central dogma; Carbohydrates; Lipids and Membranes; chemistry of drug-action.

SEMESTER – IV

Thermodynamics, chemical kinetics and electrochemistry (3:0) CORE
Laws of thermodynamics, free energies and chemical potential, applications to electrochemistry, thermodynamic properties of solids and liquids, phase equilibrium etc. Chemical reaction dynamics: rate process in chemistry, activated complex theory, photochemical reactions, chain reactions, oscillatory reactions, catalysis.

Analytical Chemistry (2:1) CORE
Errors in measurement and statistical analysis of data. Electroanalytical methods. Spectroscopic techniques of analysis and structure elucidation: atomic, IR, UV-visible, fluorescence, NMR spectroscopic methods. Separation techniques: column chromatography, GC, HPLC and hyphenated techniques. Mass spectrometry and introductory microscopy.

Inorganic Chemistry: Chemistry of Elements (3:0) CORE
Basic coordination chemistry - ligands, coordination complexes, Werner's theory - structures, isomerism, d-orbital splitting, spectrochemical series, magnetic properties. Inorganic solids: bonding, crystal systems, MOFs, supramolecular chemistry. Basic organometallic chemistry: 18-electron rule, bonding aspects, structures of organometallic compounds.

Basic Organic Reactions (3:0) CORE
Introduction to organic synthesis; Organic reactions and mechanisms: Oxidations and Reductions; Molecular rearrangements; Reactions of carbonyl compounds and unsaturated compounds; Reactions of aromatic compounds; Pericyclic reactions; Photochemistry; Radical reactions; Metal-mediated organic synthesis.

SEMESTER – V

Quantum chemistry and Statistical Mechanics (3:0)
Quantum mechanics: postulates, measurements, operators, exactly solvable problems - particle on a ring, sphere, rigid rotor, harmonic oscillator, hydrogenic atom, approximate methods. Many electron atoms and molecules: Independent particle approximation, central field problem, approximate methods for molecules, Huckel model, CNDO and semi-empirical methods, role of electron correlations. Statistical Mechanics: Ensembles, partition functions, averages, distributions, application to rotational and vibrational problems, specific heats of solids, phase transitions. Dynamics: Kinetics and relaxation, diffusion equation, non-equilibrium thermodynamics light scattering. Simulations: Configuration averages, central limit theorem, metropolis method, molecular dynamics, simulations of different ensembles.

Organic chemistry I (3.0)
Important electronic effects in organic compounds, aromaticity, frontier orbital theory, steric effects, stereochemistry, conformational analysis. Methods of

deducing organic reaction mechanisms, Hammond postulate, Curtin - Hammett principle, linear free energy relationship, Hammett and Taft equations. Organic transformations and molecular rearrangements. Reactive intermediates, classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes, arynes radical ions, diradicals, concerted reactions, Woodward-Hoffmann rules.

Inorganic chemistry I (3.0)

Main Group Chemistry: Hydrogen and its compounds, the boron and the carbon groups, the nitrogen and the oxygen groups, the halogens and noble gases. Coordination Chemistry: bonding theories- CFT, LFT and MOT, Nephelauxetic effect, magnetism and electronic spectra. Inorganic reactions and mechanisms: Hydrolysis reactions, trans-effect, isomerisation reactions, redox reactions and mixed-valence systems. Chemistry of lanthanides and actinides.

Organic & Inorganic Chemistry Laboratory (2:0)
Common organic transformations such as esterification, Diels-Alder Reaction, oxidation-reduction, Grignard reaction, etc., isolation and purification of products by chromatographic techniques, characterization of purified products by IR and NMR spectroscopy. Synthesis of coordination complexes, preparation of compounds of main group elements, synthesis of organometallic complexes. Physico-chemical characterization of these compounds by analytical and spectroscopic techniques.

SEMESTER – VI

Group theory and spectroscopy (3:0)
Group theory: Symmetry elements and operations, products of operations, point groups, matrices and representations, reducible and irreducible character tables, great orthogonality theorem, direct product of irreducible representation. Time dependent states and spectroscopy: time-dependent perturbation theory, absorption and emission of radiation, selection rules, line shapes and widths, lasers. Vibrations and rotations of diatomic molecules: Nuclear motion in diatomics, anharmonicity, vibration - rotation interaction, potential energy functions, selection rules, rotational spectra, rovibrational spectra. Vibrations of polyatomic molecules: classical mechanics of vibrations, symmetry and normal vibrations, IR and Raman spectroscopy techniques, including resonance Raman. Electronic spectroscopy: Diatomic molecules, coupling of electronic and rotational angular momentum, analysis of vibronic and rovibronic spectra, electronic spectra of polyatomic molecules, Molecular orbitals and electronic states, electronic and vibronic selection rules, multi-photon spectroscopy. Magnetic Resonance: NMR and ESR Spectroscopy, Experimental methods and applications, structure determination, 2D NMR, NMR of solids.

Organic Chemistry II – Organic Synthesis (3:0)
Principles of selectivity and reactivity in the use of reagents for oxidation, reduction and bond forming reaction. Planning a synthesis, antithetic analysis, synthons, linear and convergent synthesis.

Inorganic chemistry II – Materials Chemistry (3:0)

Structure of solids, symmetry concepts and crystal structure; Preparative methods and characterization of inorganic solids. Crystal-defects and non-stoichometry; Phase diagrams and phase transitions and kinetics of phase transformations; Structure-property correlations in ceramics, glasses and polymers; Composites and Nanomaterials; Basics of magnetic, electrical, optical, thermal and mechanical properties of solids.

Physical and Analytical Chemistry Laboratory (4:0)
Chemical kinetics, Langmuir adsorption, chemical analysis by potentiometric and conductometric methods, cyclic voltametry, flame photometry, electronic states by UV-Visible spectroscopy, IR spectroscopy; Solid state chemistry – synthesis of solids and chemical analysis, thermogravimetry, X-ray diffraction; electrical and magnetic properties of solids. Vacuum techniques in preparative chemistry.

SEMESTER – VII

Core electives can be taken from a range of course that are currently offered within the division. The following elective courses are offered by the Chemical Sciences division:

Introduction to Quantum Mechanics

Quantum Chemistry

Crystallography for Chemists

Topics in Basic and Applied Electrochemistry

Electrochemical Energy Conversion and Storage

Photophysics and Photochemistry: Fundamentals and Applications

Laser Spectroscopy and Dynamics

Polymer Chemistry

Physical Chemistry of Materials

Concepts in Material Science – I: Electronic Properties

Concepts in Material Science – II: Structure and Microstructure

Concepts in Material Science – III: Dielectrics and Ferroelectrics

Thin Film Materials and Devices: Science and Engineering

Electron Microscopy in Material Characterization

Characterization techniques in Material Science

Functional Nanoparticles, Nanowires and Nanocomposites
Theory of Materials with Electronic Correlations
Bioinorganic and Organometallic Chemistry
Advanced Organic Synthesis
Chemistry of Biological Systems
Chemistry of the Solid State
Symmetry and Structure in the Solid State
Statistical Mechanics of Liquids and Simple Systems
Computers in Chemistry
Two-dimensional NMR spectroscopy