

# Chemistry Curriculum

## Semester 1 (AUG)

### Physical Principles (2:1)

Bohr theory, Wave Particle Duality, Uncertainty principle, Schrödinger equation, H-atom and atomic orbitals, electron spin, Pauli principle and many electron atoms. Chemical bonding: covalent and ionic bonding, valence bond theory, hybridization and resonance; molecular orbital theory. Homonuclear and heteronuclear diatomics, potential energy curves and intermolecular interactions; elements of spectroscopy, van der Waals equation of state; theory of chemical reactions.

## Semester 2 (JAN)

### Basic Inorganic Chemistry (2:1)

Multi-electron atoms – periodic trends; chemical bonding: ionic solids, CFT: d-orbital splitting, tetrahedral, square planar, cubic and octahedral crystal fields, covalent bonding; Lewis model (2 Dim); VSEPR (3 Dim) hybridization; molecular orbital theory: heteronuclear diatomics, triatomics; shapes of main group compounds; acid-base chemistry: concepts, measures of acid-base strength, HSAB.

## Semester 3 (AUG)

### Basic Organic Chemistry (2:1)

Nomenclature of organic compounds: alkanes, alkenes and alkynes; structure and reactivity. Concept of aromaticity; organic reactions – Addition reactions; Elimination reactions; substitution reactions and rearrangements. Organic reaction mechanisms; reaction intermediates and their characterization. Introduction to stereochemistry.

## Semester 4 (JAN)

### Thermodynamics and Electrochemistry (2:0) (Core for majors)

Intermolecular forces, van der Waal's interactions, Leonard-Jones potentials, hydrogen bonding. Laws of thermodynamics, state functions, thermodynamic properties of liquids and solids, state equations, phase change, thermodynamic description of mixtures,

reversible and irreversible processes, colligative properties and chemical equilibrium, thermodynamic cycles.

Activity and activity coefficients, Debye-Hückel law, Arrhenius theory, cells, Nernst equation, EMF and free energy, concentration cells, conductivity, electrode processes, Fick's laws, Electrochemical techniques.

### **Instrumental Methods of Chemical Analysis (2:1) (Core for majors and minors)**

Propagation of errors in measurement, statistical analysis of data, etc. Separation Techniques: Extraction and separation, principles of chromatography. Electroanalytical Techniques: Voltammetry and its variants, ion selective electrodes and electrochemical techniques for analysis Spectroscopic Techniques: Atomic absorption/emission, Electronic, Fluorescence, and Vibrational (IR and Raman) Spectroscopy: basic principles, operation and application to chemical problems. NMR Spectroscopy: Basic principles and operation, application of one dimensional NMR for identification of chemicals. Mass Spectrometry: Principles and Applications.

### **Inorganic Chemistry: Chemistry of Elements (2:0) (Core for majors)**

Chemistry of d-block elements: structure – coordination numbers, isomerism, chelate effect; bonding: VBT, CFT, MOT; descriptive chemistry of metals: periodic trends, chemistry of various oxidation states of transition metals, oxidation states and EMFs of groups; organometallic chemistry: 18 electron rule, metal carbonyls, metal cyclopentadienyl and arene compounds, industrial catalysts; bioinorganic chemistry: metals in biological systems, heme and non-heme proteins, metalloenzymes; main group chemistry: carbon group elements (electron precise compounds); Noble gas compounds; Chemistry of f-block elements.

### **Basic Organic Reactions (2:0) (Core for majors)**

Acids and bases: definitions, pKa, pKaH, effect of structure on acid/base strength, kinetic & thermodynamic acidity, general & specific acid/base catalysis; Reactions of alkenes and alkynes: addition of halogens, hydrogen halides & interhalogen compounds, halolactonization – Baldwin's rule & Thorpe-Ingold effect, hydration, epoxidation, dihydroxylation, ozonolysis, diol cleavage, carbenes and their reactions with olefins, hydrogenation; Reactions of carbonyl compounds: addition to carbonyls, reductions,

rearrangements & their applications, oxidations, C–C bond forming reactions involving carbonyls, Cram's rule, Felkin-Anh model; Introduction to pericyclic reactions: cycloadditions, electrocyclic reactions, FMO theory and Woodward-Hoffmann rules.

## **Semester 5 (AUG)**

### **Physical Chemistry I - Quantum Chemistry and Group Theory (3:0) (Core for majors)**

Postulates of Quantum Mechanics and introduction to operators; Exactly solvable problems Perturbational and Variational Methods, Hückel model, Many electron Atoms, Slater determinants, Hartree-Fock Variational Method for atoms; Molecular Quantum Mechanics, Symmetry and Group theory, Point Groups, Reducible and Irreducible Representations (IR), Great Orthogonality theorem, Projection operators, Applications to molecular orbitals and normal modes of vibration and selection rules in spectroscopy

### **Inorganic Chemistry -Main group and Coordination Chemistry (3:0) (Core for majors)**

Main group: hydrogen and its compounds -ionic, covalent, and metallic hydrides, hydrogen bonding; chemistry of lithium, beryllium, boron, nitrogen, oxygen and halogen groups; chains, rings, and cage compounds; Coordination chemistry: bonding theories (revision and extension), spectral and magnetic properties; inorganic reactions and mechanisms: hydrolysis reactions, substitution reactions trans-effect; isomerization reactions, redox reactions; metal-metal bonding and clusters; mixed valence systems; chemistry of lanthanides and actinide elements.

### **Organic Chemistry - Structure and Reactivity (3:0) (Core for majors)**

Kinetics and reaction mechanism, primary and secondary isotope effects, Nucleophilic substitution, stereochemistry and conformation.

### **Organic & Inorganic Chemistry Laboratory (0:1) (Core for majors)**

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 6 (JAN)**

### **Physical Chemistry II: Statistical Mechanics (3:0) (Core for majors)**

Review of thermodynamics, foundations of statistical mechanics, ensembles, partition functions, averages, distributions, and non-interacting systems. Applications to rotational and vibrational problems, specific heats of solids, classical fluids, and phase transitions.

### **Material Chemistry (3:0) (Core for majors)**

Structure of solids, symmetry concepts, crystal structure. Preparative methods and characterization of inorganic solids. Crystal defects and non-stoichiometry. Interpretation of phase diagrams, phase transitions. Kinetics of phase transformations, structure property correlations in ceramics, glasses, polymers. Composites and nano-materials. Basics of magnetic, electrical, optical, thermal and mechanical properties of solids.

### **Organic Synthesis (3:0) (Core for majors)**

Principles of selectivity and reactivity in the use of reagents for oxidation, reduction and bond forming reaction. Planning a synthesis, synthetic analysis, synthons, linear and convergent synthesis.

### **Physical and Analytical Chemistry Laboratory (0:1) (Core for majors)**

Chemical kinetics. Langmuir adsorption, chemical analysis by potentiometric and conductometric methods, cyclic voltammetry, 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 7 (AUG)**

### **Basic Organometallic Chemistry (3:0) (Core for majors)**

Structure and bonding in organo-metallic compounds – isolobal analogies, metal carbonyls, carbenes and NHC complexes, olefin and acetylene complexes, alkyls and allyl complexes, metallocenes. Major reaction types – oxidative addition, reductive

elimination, insertion, isomerization and rearrangement reactions. Catalytic reactions: metathesis, hydrogenation, allylic activation, C-C coupling reactions, C-X coupling.

In addition to the core courses, electives (in the VII and VIII semesters) can be taken from a range of courses that are currently offered within the division. The following elective courses are offered the Chemical Sciences Division:

**Group Theory and Molecular Spectroscopy**

**Physical Chemistry – I Thermodynamics, Kinetics and Electrochemistry**

**Crystallography for Chemists**

**Bio & Medicinal Inorganic Chemistry**

**Electrochemical Energy Conversion and Storage**

**Advanced Organometallic Chemistry**

**Polymer Chemistry**

**Topics in Basic and Applied Electrochemistry**

**Photophysics and Photochemistry:**

**Fundamentals and Applications**

**Thermodynamics and Statistical Mechanics**

**Quantum Chemistry**

**Chemistry of Materials**

**Symmetry and Structure in the Solid State**

**Non-equilibrium Statistical Mechanics:**

**Applications to Biological Systems**

**Solar Energy: Advanced Materials and Devices**

**Statistical Mechanics of Liquids & Simple Systems**

**Topics in Solid State Chemistry**

**Functional Molecular Materials: Theory and Applications**

**Advanced Organic Synthesis**

**Asymmetric Catalysis: From Fundamentals to Frontiers**

**Graduate Colloquium**