

COTTON COLLEGE STATE UNIVERSITY
Guwahati, Assam
DRAFT SYLLABUS

DEGREE COURSE (B.Sc.) SYLLABUS IN CHEMISTRY

SEMESTER I

Paper Code	Paper Title	L+T+P	Credits
CHM101C	Physical Chemistry I	3+0+1	4
CHM102C	Organic Chemistry I	3+0+1	4
CHM103C	Inorganic Chemistry I	3+0+1	4
CHM104C	Elective Chemistry I	3+0+0	3

SEMESTER II

Paper Code	Paper Title	L+T+P	Credits
CHM201C	Physical Chemistry II	3+0+1	4
CHM202C	Organic Chemistry II	3+0+2	5
CHM203C	Inorganic Chemistry II	3+0+0	3
CHM204C	Elective Chemistry II	2+0+1	3

SEMESTER III

Paper Code	Paper Title	L+T+P	Credits
CHM301C	Physical Chemistry III	3+0+0	3
CHM302C	Organic Chemistry III	3+0+0	3
CHM303C	Inorganic Chemistry III	3+0+3	6
CHM304C	Elective Chemistry III	2+0+1	3

SEMESTER IV

Paper Code	Paper Title	L+T+P	Credits
CHM401C	Physical Chemistry IV	3+0+2	5
CHM402C	Organic Chemistry IV	3+0+0	3
CHM403C	Inorganic Chemistry IV	3+0+1	4
CHM404C	Elective Chemistry IV	2+0+1	3

SEMESTER V

Paper Code	Paper Title	L+T+P	Credits
CHM501C	Quantum Chemistry	3+0+0	3
CHM502C	Organic Chemistry V	3+0+1	4
CHM503C	Inorganic Chemistry V	3+0+2	5
CHM504C	Elective Chemistry V	2+0+1	3

SEMESTER VI

Paper Code	Paper Title	L+T+P	Credits
CHM601C	Molecular Spectroscopy	3+0+0	3
CHM602C	Organic Chemistry VI	3+0+1	4
CHM603C	Inorganic Chemistry VI	3+0+2	5
CHM604C	Elective Chemistry VI	2+0+1	3

Semester I

Paper: CHM101C (Physical Chemistry I) Credit: 3+0+1 = 4

Unit 1: CHEMICAL THERMODYNAMICS – I 16L

Definition of thermodynamic terms: Closed, open and isolated systems; surroundings; concepts of energy and the system internal energy U , heat transfer q and work done w . The zeroth law and the concept of temperature.

The first law (with old and new notations about the work done w), calculation of work done during isothermal and adiabatic expansion of an ideal gas, thermodynamic reversibility, heat capacity, enthalpy and its significance.

State functions and differentials; variation of internal energy and enthalpy with temperature, Joule-Thomson experiment and liquefaction of gases; relation between C_p and C_v in general and for ideal gases. Relation between P , V , T for adiabatic processes in an ideal gas.

Thermochemistry – standard enthalpy changes, derivation of Hess's law and Kirchoff's law. Relation of reaction enthalpy with changes in internal energy. Calculation of bond dissociation energies from thermochemical data.

Unit 2. THE GASEOUS STATE OF MATTER 16L

Distribution of molecular speed – Maxwell's speed distribution law. Concept of mean, root mean square (r.m.s.) and most probable speeds – their expressions from the speed distribution law. Kinetic theory of gases: Postulates, expression of pressure in terms of the r.m.s. speed of gas molecules. Interpretation of the ideal gas law $PV = nRT$ in terms of the kinetic theory expression. Degrees of freedom, principle of equipartition of energy, molecular basis of the heat capacity of gases.

Collision among gas molecules: collision cross-section, collision frequency, collision density and mean free path.

Deviation from ideal behaviour of gases: van der Waals equation of state, virial equation of state, critical phenomena, equation of corresponding states.

Concepts of transport properties of gases, flux and the Fick's law of diffusion. Rate of diffusion, thermal conductivity and coefficient of viscosity of a gas; relations for these three transport properties without derivation.

Unit 3: CHEMICAL KINETICS 16L

Concept of reaction rate and rate laws. Order and molecularity of reactions. Differential rate equations and integrated rate expressions for zero, first and second order reactions. Half-life periods and their dependence on initial concentrations. Temperature dependence of reaction rates, Arrhenius plots.

Consecutive, concurrent and opposing reactions. The steady state approximation and the rate determining step approximation; kinetics of decomposition of N_2O_5 . Experimental determination of rate and order of reactions: various methods and techniques.

Kinetics of chain reactions, $\text{H}_2\text{-Br}_2$ reaction, thermal decomposition of ethanal, branching and non-branching chain reaction, $\text{H}_2\text{-O}_2$ reaction, concept of explosion limits. Introduction to polymerisation kinetics of free-radical chain polymerisation.

Unit 4: PHYSICAL CHEMISTRY PRACTICAL (1 Credit)

- Determination of the concentrations of sodium carbonate and sodium hydroxide in a mixture of the two in aqueous solution.
- To determine the solubility of a given substance at different temperatures and to plot the solubility curve.
- Determination of equivalent mass of an acid (e.g., oxalic acid) by direct titration method.

Paper: CHM102C (Organic Chemistry I) Credit: 3+0+1 = 4

Unit 1: INTRODUCTION TO ORGANIC COMPOUNDS 10 L

Classification of organic compounds. IUPAC nomenclature for organic compounds with single and multiple functional groups including bicyclo compounds, spirans etc.

Unit 2: ORGANIC STRUCTURE AND ACTIVITY 10 L

Hybridisation, bond lengths, bond angles and bond energies. Concept of localised and delocalised chemical bonds, inductive, field, resonance and hyperconjugative effects. Huckels rule and aromaticity. Hydrogen bonding and its effect on molecular properties.

Lewis and Bronsted-Lowry concepts of acids and bases. Effect of structure on acidic and basic properties of organic compounds.

Unit 3: ORGANIC STEREOCHEMISTRY – I 12 L

Constitutional isomerism vs Stereoisomerism. Types of stereoisomerism – configurational and conformational isomers, enantiomers and diastereomers. Geometrical isomerism and the π -diastereomers. Cis-Trans, syn/anti and E-Z nomenclatures. Differences in physical and chemical properties of the π -diastereomers.

Optical isomerism, chirality or dissymmetry, asymmetry. Designation of Configuration: R/S system, Fischer Projection formula. Racemic mixtures, resolution of racemic mixtures.

Conformation of acyclic systems with examples of ethane and butane, nomenclature for the conformers. Newman and Sawhorse projection formula for the conformers.

Unit 4: ORGANIC REACTION MECHANISMS – I 16 L

Activation energy and transition state. Energy profile diagram for reactions with single or multiple steps. Concepts of kinetic and thermodynamic control. Stereospecific and stereoselective reactions.

Notations used in reaction mechanisms. Types of reagents: electrophiles and nucleophiles. Types of reaction intermediates: carbocations (including non-classical types), carbanions, carbenes and nitrenes. Methods for determination of reaction mechanisms.

Addition reactions: electrophilic, nucleophilic and free radical mechanisms.

Unit 5: ORGANIC CHEMISTRY PRACTICAL (1 Credit)

1. Chromatography:

- (a) Paper chromatographic separation and identification of sugars
- (b) Thin layer chromatographic separation of pigments from leaves and flowers

2. The following preparations are to be done by each student in class. Any one of these will be required to be done in the examination.

(a) Acetylation or benzylation: Preparation of acetanilide or benzanilide from aniline

(b) Nitration: Preparation of m-dinitrobenzene from nitrobenzene OR preparation of p-nitro acetanilide from acetanilide.

Students should recrystallise the prepared product and determine the melting point.

Paper: CHM103C (Inorganic Chemistry I) Credit: 3+0+1 = 4

Unit 1: FUNDAMENTALS OF ATOMIC STRUCTURE 16L

The defining limit of classical mechanics – the uncertainty principle. Necessity of the quantum mechanical approach for sub-microscopic systems.

Schrodinger equation - statement and identity of terms. Energy eigenvalues – expression alone. Energy eigenfunctions: Setting-up of expressions of radial (R) and angular (Y) parts for 1s, 2s, 2p_o, 2p₊₁, 2p₋₁, 2p_z, 2p_x, 2p_y orbitals, Born interpretation of the wave functions.

Concept of orbital as one-electron wave functions. Plots of $|\Psi|$ and $|\Psi|^2$ for 1s, 2s, 2p_x, 2p_y, 2p_z orbitals. The quantum numbers n, l, m_l – origin and significance (outline only).

The concept of spin and the spin quantum numbers s and m_s (outline only).

Many electron atoms: inter-electronic repulsion in the He atom. Pauli's exclusion principle. Hund's rule.

Effective nuclear charge – shielding and penetration effects, Slater's rules, Order (ranking) of atomic-subshell (1s, 2s, 2p, 3s, 3p....) energies for many-electron atoms. Aufbau principle and electron configuration of many electron atoms.

Unit 2: CHEMICAL BONDING – I 16L

Lewis electron pair bond. Valence bond approach to bonding in diatomic molecules – outline of the concept of orbital overlap (in HF and H₂).

Resonance and resonance energy.

Bond moments and dipole moments (outline with simple pictorial representation).

Percent ionic character of HCl and HF bonds. Dipole moment of molecules.

Formal charges on atoms in molecules.
Concept of electronegativity – explanation of molecular properties on the basis of electronegativity.
Shapes of molecules – VSEPR theory, hybrid orbitals and hybridisation in polyatomic molecules – influence of hybridisation on bond length, bond angle and other properties of molecules including shapes and dipole moments. Effects of structure on molecular properties – steric effects and electronic effects.

Unit 3: CHEMICAL BONDING – II 16L

Molecular orbital theory of common homonuclear and heteronuclear diatomic molecules (H_2 , N_2 , O_2 , F_2 , NO and CO).

Graphical representation of angular parts of the wave function (H_2^+ molecular ion). Electronic configurations of ground states of diatomic molecules with energy-level diagrams. Setting up of the wave functions and energy level diagrams for molecules without calculations.

Multicentre bonding (as in diborane); MOs of simple triatomic systems (BeH_2 , H_2O), Bond energy, bond length and covalent radii.

Bonding in metals (band theory); properties consequent from band theory.

Unit 4: INORGANIC CHEMISTRY PRACTICAL (1 Credit)

- (a) To determine the water of crystallization of a hydrated salts (e.g., blue vitriol) by ignition and weighing.
- (b) To determine the total hardness of water by titration with EDTA.
- (c) To determine the water of crystallization of green vitriol by titration of its prepared solution with $KMnO_4$ solution.

Semester II

Paper: CHM201C (Physical Chemistry II)

Credit: 3+0+1 = 4

Unit 1: CHEMICAL THERMODYNAMICS – II

16 L

The unidirectional nature of spontaneous processes. The second law and the concept of entropy. Entropy changes in reversible and irreversible processes, Clausius inequality. Calculation of entropy changes during various processes in ideal gases.

Helmholtz function and Gibbs function and the direction of spontaneous change. Thermodynamics of chemical reactions. Equilibrium constant of a reaction in terms of standard Gibbs function; dependence of equilibrium constant on temperature and pressure.

Standard enthalpy, entropy, and Gibbs function of a reaction; standard enthalpy and Gibbs function of formation. Maxwell's relations and the derivation of thermodynamic equation of state; Gibbs-Helmholtz equation, variation of Gibbs function with pressure and temperature.

Concept of partial molar quantities; definition and brief idea about chemical potential: Expression relating it with the Gibbs function (i.e., $G = \sum_i n_i \mu_i$), the Gibbs-Duhem equation and its derivation.

The Nernst heat theorem and third law of thermodynamics.

Unit 2: ELECTROCHEMISTRY – I

12 L

Electrochemical cells: measurement of e.m.f. and electrode potentials, concept of SHE, electrode-potential sign convention, different classes of electrodes, the calomel electrodes (SCE, NCE and DNCE) and their use as reference electrodes. Nernst equation. Equilibrium constants and activity coefficients from standard electrode potentials. Chemical cells and concentration cells, cells with and without transference.

Primary cells: construction and working of zinc-graphite dry cells (acidic and alkaline). Secondary cells: construction and working of lead-acid battery. Fuel cells, their applications and reason behind their high efficiency. Electrochemical basis of corrosion in metals, prevention of corrosion.

Unit 3: LIQUIDS AND COLLOIDS

12 L

Structure of liquids (qualitative treatment) – structure of liquid water and ice. Physical properties of liquids: vapour pressure, surface tension and viscosity. Determination of surface tension and the coefficient of viscosity of a liquid.

Liquid crystals: elementary idea of structure, physical properties and uses of liquid crystals.

Colloids: Definition, sols and lyophilic colloids; preparation and purification of colloids, structure, surface and stability of colloids, Surface-active agents (surfactants), micelle formation, critical micellar concentration (CMC), electrical double layer and electrokinetic phenomena.

Unit 4: COLLIGATIVE PROPERTIES

8 L

Raoult's law and Henry's law. Definition of colligative property: lowering of vapour pressure, boiling point elevation, freezing point depression, osmotic pressure -- numerical calculations based on colligative property measurements. Abnormal colligative properties due to dissociation and association, van't Hoff factor.

Thermodynamic treatment of colligative properties. Real solutions: activity and activity coefficient.

Unit 5: PHYSICAL CHEMISTRY PRACTICAL (1 Credit)

- (a) To determine the composition of a given aqueous solution by viscosity measurements.
- (b) To determine the composition of a given aqueous solution by surface tension measurements.
- (c) To determine the concentration of an optically active substance in solution and also its specific rotation by polarimetric measurements.

Paper: CHM202C (Organic Chemistry II) Credit: 3+0+2 = 5

Unit 1: ORGANIC REACTION MECHANISMS – II 20 L

Substitution reactions:

a) Nucleophilic aliphatic substitution – S_N1 and S_N2 and S_Ni reactions. Factors influencing the S_N1 and S_N2 pathways. Walden inversion.

b) Mechanism of electrophilic aromatic substitution. Directive influence of groups, activation and deactivation of aromatic rings, o/p ratio, mechanism to be given with examples.

Elimination reaction

Base catalysed and pyrolytic Elimination, Elimination vs. substitution reactions – controlling factors. : Saytzeff and Hoffmann elimination.

Unit 2: CLASSES OF ORGANIC COMPOUNDS – I 10 L

Alkanes: Preparation of alkanes with special reference to Wurtz reaction, Kolbe's reaction and Corey-House reaction. Physical properties and reactivities of alkanes. Mechanism of halogenation, relative reactivities towards halogenation, principle of reactivity and selectivity.

Cycloalkanes: Bayer strain theory and its limitations. Angle strain, banana bond in cyclopropane ring. Shapes of cyclopentane and cyclohexane rings.

Unit 3: CLASSES OF ORGANIC COMPOUNDS – II 9 L

Alkyl halides: Preparation, physical properties and reactions. Grignard and organolithium reagents.

Alcohols: Preparation with special reference to hydroboration and oxymercuration. Conversions to and from alcohols. Properties.

Glycols and their reactions with lead tetra-acetate and per-iodic acid.

Unit 4: CLASSES OF ORGANIC COMPOUNDS – III 9 L

Alkenes: Preparation of alkenes with special reference to dehydrohalogenation and dehydration of alcohols.

Properties of alkenes with special emphasis on addition to C=C bond. Markownikoff's rule.

Addition of HBr to alkenes. Peroxide effect. ozonolysis and hydroxylation by KMnO_4 are to be emphasised. Reactivities of vinylic and allylic hydrogen atoms in alkenes.

Alkynes: Methods of formation of alkynes, reactivity of alkynes, metal acetylides.

Unit 5: ORGANIC CHEMISTRY PRACTICAL (2 Credits)

Qualitative analysis of organic compounds (liquids or solids) and identification by:

- Detection of nitrogen, sulphur and halogens.
- Test for functional groups by analytical methods.
- Solubility and melting point/ boiling point
- Preparation of a derivative and determination of its melting point.

(At least five organic compounds must be analysed during the session)

Paper: CHM203C (Inorganic Chemistry II) Credit: 3+0+0 = 3

Unit 1: CHEMISTRY OF NON-TRANSITION ELEMENTS – I 16L

Polarizing power of cations. Polarisability of anions, Fajan's rules and its consequences.

Non-aqueous solvents: liquid ammonia, liquid sulphur dioxide, liquid HF, liquid N_2O_4 and supercritical CO_2 .

Preparation, properties, bonding and structure of the following:

- Ortho and para hydrogen, hydrates, clathrates and inclusion compounds.
- Allotropes of carbon (including fullerenes), graphene, intercalation compounds, carbides, cyanogens, oxides and oxy-acids of carbon.

Unit 2: PROPERTIES OF INORGANIC COMPOUNDS 16L

The long form of the periodic table – general discussion.

Detailed discussion of the following properties of main group elements (1-2, 13-18):

- Electronic configuration, size of atoms, ions and atomic orbitals.
- Ionisation energy and electron affinity of atoms.
- Tendency to use vacant d-orbitals and electropositive character of metals.
- Electronegativity of elements – Pauling, Mulliken, Alred-Rachou and Mulliken-Jaffe's electronegativity scales, variation of electronegativity with bond order, partial charge, hybridisation, group electronegativity, electroneutrality principle.
- Melting point and boiling point of elements and their compounds.
- Solubility of salts and molecules in water.
- Bronsted-Lowry concept of acids and bases: relative strengths of acids, amphoterism, levelling solvents, pH and pK_a , buffer solutions. Lewis concept of acids and bases: classification of Lewis acids. Hard and soft acids and bases (HSAB) principle, application of HSAB principle.
- Catenation and inert-pair effect.

(i) Electrode potentials and redox behaviour in aqueous solutions. The Latimer diagram and Frost diagram, their uses.

Unit 3: CHEMISTRY OF NON-TRANSITION ELEMENTS – II

16L

Allotropes of phosphorous. Hydrides, oxides and oxy-acids of nitrogen and phosphorous. Hydrazine, hydroxylamine and hydrogen azide, clinical use of NO and N₂O

Superoxide and oxygen fluorides. Allotropes of sulphur. oxides, hydrides, oxyacids and per-acids of sulphur.

Interhalogen compounds, polyhalides, pseudohalogen, oxides and oxyacids of halogens.

Noble gas compounds – xenon oxides and fluorides.

Inorganic chains, ring and cages: Silicate, aluminosilicates, zeolites, silicones, borazine, phosphazine, S₄N₄, P₄, P₄O₆, P₄O₁₀, diborane, boron cage compounds, carboranes and metallocarboranes.

Semester III

Paper: CHM301C (Physical Chemistry III) Credit: 3+0+0 = 3

Unit 1: PHASE EQUILIBRIA 18L

Definition of phase, meaning of components and degrees of freedom, derivation of phase rule. Phase diagram of one component systems (water, sulphur). Phase diagram of two-component systems (eutectics, congruent and incongruent melting points, solid solutions)

Interpretation of liquid-vapour, liquid-liquid and liquid-solid phase diagrams, distillation of liquid solutions and immiscible liquid mixtures.

Clausius-Clapeyron equation for different phases. Systems of variable composition, partial molar quantities, Gibbs-Duhem equation, thermodynamics of mixing.

Chemical potentials - chemical potential of a component in an ideal mixture – fugacity, activity, activity coefficients. Dependence of chemical potential on temperature and pressure.

Unit 2: DATA ANALYSIS 15L

Errors and deviations in measurements of physical quantities: accuracy and precision. Absolute, relative and mean errors. Relative and mean deviation, standard deviation. Significant figures in reporting measurements and calculation results, its relation to precision. Types of errors: determinate and indeterminate errors, various types of determinate errors.

Propagation of errors in calculations. Uncertainty in measurement of physical quantities and in universal constants.

Linear least-square fitting of experimental data-points.

Reliability of Results (Q Test), Confidence Interval. Comparison of Results – Student's t Test and F Test.

Unit 3: ELECTROCHEMISTRY II 15L

Ion transport and conductivity, mobility of ions and conductivity. Concept of current density and of electric field strength – their interrelation. Transport number of ions and methods for their determination. Conductance, conductivity, molar conductivity and equivalent conductivity, Kohlrausch's law of independent migration of ions. Dependence of molar conductivity on concentration and temperature - the Debye-Huckel-Onsagar equation. Activity of ions, mean ionic activity, ionic strength of solutions, Debye-Huckel theory (elementary ideas only) of strong electrolytes.

Strong and weak electrolytes, dissociation equilibria of weak electrolytes, Ostwald's dilution law. Concept of pK_a and pK_b of acids and bases. Henderson-Hasselbalch equation. Buffer solutions and buffer action.

Paper: CHM302C (Organic Chemistry III)

Credit: 3+0+0 = 3

Unit 1: ORGANIC STEREOCHEMISTRY – II

9 L

Conformation of cyclohexane: boat and chair forms. Axial and equatorial positions, isomerism in disubstituted cyclohexane.

Concept of topicity and prostereoisomerism. Criteria of establishing topicity of groups, atoms and faces. Designation of stereoheterotopic atoms, groups and faces.

Unit 2: CLASSES OF ORGANIC COMPOUNDS – IV

10 L

Carbonyl compounds: Preparation of carbonyl compounds. Nucleophilic addition to carbonyl compounds – redox reactions and condensation reactions. Mechanisms of aldol condensation, Cannizzaro reaction, Claisen condensation, Reformatsky reaction,

Oppeneauer reaction, Wolff-Kishner reduction, Benzoin condensation, Perkin reaction, Knoevenagel condensation, Wittig reaction, Beckmann rearrangement.

Unit 3: CLASSES OF ORGANIC COMPOUNDS – V

9 L

Carboxylic acids and their derivatives: Preparation of carboxylic acids, physical properties, acidity and effect of substituents. Derivatives of carboxylic acids – acid chlorides, amides and esters. Acidic and alkaline hydrolysis of esters.

Dicarboxylic acids – oxalic, malonic and succinic acids. Hydroxy acids and unsaturated acids

Unit 4: CLASSES OF ORGANIC COMPOUNDS – VI

10 L

Ethers: preparation, cleavage and auto-oxidation reactions. Epoxides: preparation, acid and base catalysed ring opening.

Amines (aliphatic and aromatic): Classification and preparation of amines, distinction between primary, secondary and tertiary amines. Hoffmann bromamide reaction, exhaustive methylation and Hoffmann elimination, Hinsberg test, carbylamine test, Mannich reaction. Formation of diazonium salts, uses of diazonium salts. Sandmeyer reaction. Quaternary ammonium salts.

Unit 5: CLASSES OF ORGANIC COMPOUNDS – VII

10 L

Phenols: Preparation and typical reactions. Fries rearrangement, Kolbe's reaction, Reimer-Tiemann reaction (with mechanism).

Haloarenes: Preparation, mechanism of nucleophilic aromatic substitution, benzyne mechanism, cine substitution, chichibabin reaction and methods of trapping benzyne intermediates.

Paper: CHM303C (Inorganic Chemistry III)

Credit: 3+0+3 = 6

Unit 1: SYMMETRY AND POINT GROUP OF MOLECULES

12L

Symmetry elements and symmetry operation, concept of point group, point groups of simple molecules, symmetry of octahedron, tetrahedron and square planar complexes, structure and symmetry of inorganic compounds (coordination number 2-6), shape and symmetry of s, p, and d orbital.

Representation of symmetry operators by matrices, representation of groups – reducible and irreducible representation. Character tables of C_{2v} and C_{3v} point group.

Unit 2: SOLIDS

18L

Types of solids. Types of unit cells; crystal lattices and Miller indices; crystal system and Bravais lattices for elemental crystals. Close-packed structures of elemental solids.

Ionic solids: ionic radii; radius ratio and its effect on structures of binary ionic crystals. Structures of common binary ionic crystals – CsCl structure, NaCl structure, both ZnS structures, fluorite structure. Common ternary ionic crystals: spinel and perovskite structures. Lattice energy of ionic solids; Born-Haber cycle calculations.

Dislocation in solids, Schottky and Frenkel Defects.

Electrical property of solids (conductor, insulator, intrinsic and extrinsic semiconductors, n-type and p-type semiconductors), super conducting materials.

Unit 3: COORDINATION COMPOUNDS

18L

Coordination Compounds: Werner's theory, EAN rule, structural and stereoisomers of complex compounds, survey of different types of ligands, IUPAC nomenclature of coordination compounds. Structure and bonding (valence bond theory) of complexes containing the following as one of the ligands: CO, CN, CH_3COO^- , $C_2O_4^{2-}$, NH_3 , en, acac, Metal Carbonyls and Nitrosyls.

Unit 4: INORGANIC CHEMISTRY PRACTICAL

(3 Credit)

Qualitative Inorganic Analysis: Analysis of mixture of two inorganic salts containing total of four cations and anions including insoluble salts and interfering anions.

(At least eight such mixtures of inorganic salts must be analysed during the session)

Semester IV

Paper: CHM401C (Physical Chemistry IV)

Credit: 3+0+2 = 5

Unit 1: MOLECULAR REACTION DYNAMICS

18L

Collision theory, Activated complex theory, Eyring equation – thermodynamic formulation. Theory of unimolecular reactions (Lindemann theory) – dynamic molecular collisions – potential energy surfaces. Molecular beam technique and results of molecular beam studies.

Reactions in solution, Bronsted-Bjerrum equation, Kinetic salt effect. Laws of photochemical equivalence, quantum yield. Kinetics of $\text{H}_2\text{-Br}_2$, $\text{H}_2\text{-Cl}_2$ reactions, dissociation of HI. Photo-stationary equilibrium, dimerisation of anthracene.

Luminescence phenomenon: fluorescence, phosphorescence, Jablonski diagram, photosensitised reactions, quenching of fluorescence. Chemiluminescence and bioluminescence. Introduction to lasers and flash photolysis.

Photochemistry of air and air pollution.

Unit 2: SURFACE CHEMISTRY AND CATALYSIS

12L

Introduction to solid surfaces, adsorption at surfaces – physisorption and chemisorption. Adsorption isotherms – Langmuir and BET isotherm and their derivation. Determination of surface area using adsorption isotherms. Catalytic activity at surface with examples. Concept of surface excess, Gibbs isotherm relating surface excesses.

Homogeneous catalysis: oxidation of SO_2 to SO_3 catalysed by NO, acid-base catalysis, enzyme catalysis with Michaelis-Menten equation. Effect of pH and temperature on enzyme catalysis. Heterogeneous catalysis: zeolites and their use as catalysts in cracking of petroleum.

Unit 3: STATISTICAL AND NON-EQUILIBRIUM THERMODYNAMICS

18L

Molecular energy levels and concept of distribution of gas molecules in energy levels. Concept of macrostate (thermodynamic state) and microstate (quantum mechanical state) for a gaseous system. Molecular significance of heat and work.

The Boltzmann distribution in a gaseous system, the molecular partition function and its significance. Translational, electronic, rotational and vibrational partition functions of gas molecules. Statistical thermodynamics of monatomic and diatomic gases.

Applications of statistical thermodynamics for calculation of equilibrium constants of gaseous reactions.

Non-Equilibrium thermodynamics: Concept of internal production in irreversible processes. Generalised forces and flows, phenomenological relations, statement of Onsager's reciprocal relation.

Unit 4: PHYSICAL CHEMISTRY PRACTICAL

(2 Credit)

- To determine the concentration of an aq. HCl solution by conductometric titration versus aq. NaOH solution standardised using an oxalic acid solution.
- To determine the concentration of an aq. CH_3COOH solution by pH-metric titration versus aq. NaOH solution standardised using an oxalic acid solution.
- To determine the mutual solubility curve of phenol and water.

- (d) To determine the rate constant of hydrolysis of methyl acetate catalysed by a strong acid at room temperature.
- (e) To obtain Freundlich isotherm for adsorption of oxalic acid on activated charcoal.
- (f) To verify the Lambert-Beer's law for a coloured solution of KMnO_4 / $\text{K}_2\text{Cr}_2\text{O}_7$ / CuSO_4 using spectrophotometer.
- (g) Determine the composition of iron(III)-thiocyanato complex spectrophotometrically by Job's method of continuous variation

Paper: CHM402C (Organic Chemistry IV) Credit: 3+0+0 = 3

Unit 1: OXIDATION AND REDUCTION REACTIONS 20 L

Use of common oxidising agents namely: chromium trioxide, selenium dioxide, PCC, lead tetra acetate, chromyl chloride, permanganate, per iodine acid, osmium tetroxide. Mechanism of the oxidation reactions. Typical oxidation reactions – Oppenauer oxidation, Swern oxidation, Des-Martin oxidation.

Mechanism of reduction reactions occurring through:

- (i) Direct electron transfer – e.g., Clemmensen reduction (Nakabayashi mechanism), Birch reduction
- (ii) Hydride transfer – Use of LiAlH_4 and NaBH_4 , MPV reduction.
- (iii) Hydrogen atom transfer – Boveault-Blanc reduction.
- (iv) Catalytic reduction (hydrogenation with Pd, Pt and Raney Ni)
- (v) Selective reduction – Rosenmund reduction, use of Lindlar's catalyst

Unit 2: BIOCHEMISTRY – I 20 L

Proteins: α -amino acids, essential and non-essential amino acids, peptide bonds, peptides and polypeptides. Structure of proteins: Primary, secondary, tertiary and quaternary structure.

General ideas of nucleosides, nucleotides and nucleic acids, purine and pyrimidine bases. Concept of base pairing.

Lipids: definition, structure of cell membrane, lipid bilayer, transport through membranes.

Carbohydrates: Classification and general study of the properties of carbohydrates. Interrelationship among the monosaccharides, configuration of the hydroxyl groups in the monosaccharides. Structure of glucose and fructose. Mutarotation of glucose.

Unit 3: INTRODUCTION TO GREEN CHEMISTRY 8 L

Green chemistry: Concept, basic principles of green chemistry. Concepts of waste prevention, safer chemicals, renewable feedstock, preference for catalysts, atom economy, safer solvents and solvent-less operations. Applications: modern (BHC) synthesis of ibuprofen and microwave-assisted Friedel-Crafts reaction.

Paper: CHM403C (Inorganic Chemistry IV) Credit: 3+0+1 = 4

- Unit 1: BONDING IN COORDINATION COMPOUNDS 13 L
Crystal field theory, factors affecting $10 Dq$ value, crystal field stabilization energy, magnetic properties from crystal field theory, spectrochemical series, nephelauxetic effect, high spin and low spin complexes, Jahn-Teller distortion, structural and thermodynamic effects of orbital splitting, octahedral versus tetrahedral coordination in spinels. Adjusted crystal field (i.e., ligand field) theory, Molecular orbital theory of octahedral complexes (without and with π bonding).
Metal-metal bonding and quadrupole-bonds.
- Unit 2: ANALYTICAL TECHNIQUES IN INORGANIC CHEMISTRY 10L
Electroanalytical techniques: voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry.
Thermogravimetric techniques: TGA, DTA, DSC, online analyser.
Application of atomic and molecular absorption and emission spectroscopy in quantitative analysis.
- Unit 3: CHEMISTRY OF METALS 12 L
Bonding in metals, physical and chemical properties of metals.
Occurrence and principles of extraction of Ni, Fe, Cu, Zn and Al.
Physical and chemical properties of ionic compounds of alkali metals, alkaline earth metals and aluminium.
Allotropes of tin, inert pair effect in Sn, Pb and Tl.
Zn, Cd, Hg: Stereochemistry of compounds, the mercurous ion, divalent compounds, coordination complexes.
- Unit 4: NUCLEAR CHEMISTRY 13 L
Structure of the nucleus, Nuclear Models (Liquid Drop, Shell), Nuclear Forces, Nuclear Stability, mass defect and binding energy. Types of Nuclear reactions, Q value, nuclear cross sections, Fission, Fusion, Nuclear Reactors.
Radioactivity, Theory of radioactive disintegration, Radioactive decay and equilibrium, Rates of disintegration, the radiochemical series. Transmutation of elements and artificial radioactivity.
Isotopes of elements, methods of separation of isotopes, application of isotopes (tracer technique, neutron activation analysis, radiocarbon dating).
- Unit 5: INORGANIC CHEMISTRY PRACTICAL (1 Credit)
Preparation of the following compounds:
1. Chrome alum
2. Tetramine Cu(II) sulphate
3. Hexammine Ni(II) chloride
4. Mohr's salt
5. Potassium trioxalato chromate(III)
Students should recrystallise the prepared product and verify the presence/ absence of anions and cations, as are applicable, by qualitative analysis.

Semester V

Paper: CHM501C (Quantum Chemistry) Credit: 3+0+0 = 3

Unit 1: BASIC IDEAS OF QUANTUM MECHANICS 16L

Wave functions – operators, eigenfunctions and eigenvalues. The basic postulates of quantum mechanics. Schrodinger wave equation – time dependent and time independent forms. Concept of boundary conditions. Born interpretation and normalization of the wave function – orthogonal and orthonormal wave functions. Expectation values of physical observables and their calculations.

Cartesian and spherical polar coordinate systems, construction of Hamiltonian with potential function leading to potential energy term.

Model systems – particle in 1-D, 2-D and 3-D boxes, particle in a ring, harmonic oscillator and rigid rotor (detailed mathematical treatment not necessary). Outline of solution of their Schrodinger equations, energy expression, wavefunctions and quantum numbers.

Qualitative discussions of special features like degeneracy, energy level diagrams, quantum mechanical tunnelling, force constant and zero point energy for harmonic oscillator, moment of inertia in 3D, angular momentum, space quantization of angular momentum for rigid rotor.

Unit 2: ATOMIC STRUCTURE AND ATOMIC SPECTRA 16L

The Hamiltonian and Schrodinger equation for hydrogen and helium atoms, energy levels and quantum numbers, the radial and angular part of the wave functions, concept of atomic orbitals. Plots of atomic-orbital wave functions and their squares vs. displacement from origin, construction of two-dimensional plots of probability density and calculation of radial probability functions. The orbitals of hydrogen and hydrogen-like atoms, contour diagrams of electron probability density.

Electron spin and spin quantum number – spin orbitals, Stern-Gerlach experiment. Electron configuration of many electron atoms, Pauli's exclusion principle – illustration by He atom. Wave functions of many electron atoms. Effective nuclear charge and Slater's rules.

Electronic transitions and the spectrum of atomic hydrogen, Spectral selection rules. Spectra of complex atoms, States derived from electron configurations, Hund's rules, Spin - orbit interactions, Russel-Saunders coupling, term symbols, and effect of magnetic field on energy levels.

Unit 3: THE NATURE OF THE CHEMICAL BOND 16L

Quantum theory of the electron pair bond (Heitler-London theory), potential energy curve of the hydrogen molecule. The concept of resonance and electronegativity from VB theory, the overlap criterion of bond strength, construction of hybrid orbitals.

The LCAO approximation in MO theory. Molecular orbital energy level diagram for homonuclear (H_2^+ , H_2 , O_2 , N_2) and heteronuclear (HF, LiF, CO) diatomic molecules. Representation of polarity of bonds in the MO theory and VB theory, term symbols of diatomic molecules, origin of term symbols.

Huckel MO theory for 1,3-butadiene, 1-3-cyclobutadiene and for benzene. Justification of the Huckel $(4n+2)$ rule.

Paper: CHM502C (Organic Chemistry V) Credit: 3+0+1 = 4

- Unit 1: MOLECULAR REARRANGEMENTS 10 L
(i) Nucleophilic or anionotropic rearrangements: Wagner-Meerwein rearrangement, Whitmore 1,2-shift, Wolff, Curtius, Hoffmann, Lossen, Beckmann, Benzil-benzilic acid, Baeyer-Villiger rearrangements.
(ii) Electrophilic or cationotropic: pinacol rearrangement.
(iii) Free radical: Wittig rearrangement.
(iv) Special rearrangements: Fries rearrangement, Stevens rearrangement, Cope and Claisen rearrangement.
- Unit 2: CLASSES OF ORGANIC COMPOUNDS – VIII 8 L
Polynuclear Aromatic Hydrocarbons: Structure, bonding, properties and important derivatives of naphthalene, anthracene and phenanthrene.
Nitro and cyano compounds: Synthesis, physical properties and reactivity of nitroalkanes, alkyl nitrates, alkyl nitriles, isonitriles and aromatic nitro compounds.
- Unit 3: ORGANIC POLYMERS 12 L
Polymers and polymerisation reactions: Chain (addition) and step-reaction (condensation) polymerisation. Classification of polymers as (a) plastics, fibres and elastomers, and as (b) thermoplastic and thermosetting polymers.
Synthesis of polythene, PVC, poly acrylonitrile, PET (terylene) and nylon.
Structure of natural rubber; structure, synthesis and use of Buna-S synthetic rubber.
Thermosetting polymers: structure and use of UF (urea-formaldehyde) and PF (phenol-formaldehyde) resins.
Molecular weight of macromolecules, number average and mass average molecular weight. Determination of molecular weight of macromolecules: Viscometry and Osmometry (basic ideas only).
Biopolymers: polysaccharides (cotton etc.) and polypeptides (wool etc.),
- Unit 4: BIOCHEMISTRY – II 10 L
Biosynthesis of DNA (replication), of RNA (transcription) and of proteins(translation).
Enzymes and their classification. Metalloenzymes and coenzymes.
Hormones: Definition, classification and basic functions.
Fundamentals of biological energy production: Glycolysis, Kreb's cycle.
Respiration, oxidative phosphorylation and ATP synthesis. Photosynthesis.
- Unit 5: PERICYCLIC REACTIONS 8 L
Definition and examples of $(2+2)$ and $(2+4)$ cycloadditions, $(1+3)$ dipolar cycloadditions.
Conservation of orbital symmetry – Woodward-Hoffmann rules.

Electrocyclic reactions – HOMO-LUMO approach. Sigmatropic rearrangements.

Unit 6: ORGANIC CHEMISTRY PRACTICAL (1 Credit)

Organic quantitative analysis:

- Determination of equivalent mass of an acid by titrimetric method.
- Determination of amount of glucose by titration with Fehling's solution.
- Determination of saponification number of an ester.

Paper: CHM503C (Inorganic Chemistry V) Credit: 3+0+2 = 5

Unit 1: MAGNETOCHEMISTRY 12L

Magnetic properties of free metal ions, spin-only magnetic moments of d^n ions in weak and strong crystal fields of O_h and T_d symmetries. Orbital contribution and the effect of spin-orbit coupling, quenching of orbital angular momentum by crystal fields, ferromagnetism and anti-ferromagnetism with examples from metal complexes. Magnetic properties of second and third transition series and lanthanide elements.

Unit 2: BIOINORGANIC CHEMISTRY 18L

Essential and trace elements and their biological role, importance of Na^+ and K^+ ions in biology; Na-K pump. Biochemistry of Ca^{2+} ions.

Uptake and storage of iron, structure and function of haemoglobin and myoglobin, cytochromes, peroxidases, catalases. Ferritin and transferrin.

Nitrogen fixation and photosynthesis in plants.

Inorganic medicinal compounds: cis-platin and related complexes, vanadium complexes, importance of nitric oxide in biochemistry.

Toxicity due to metal ions (Hg, Pb, Cd, As). Nitrogen oxides and photochemical smog. Ozone layer and its depletion. The green house effect.

Importance of metal salts in human diet.

Unit 3: ORGANOMETALLIC COMPOUNDS 18L

Classification, IUPAC nomenclature. Effective atomic number rule, Synthesis, structure and bonding of complexes with olefins, alkyl, allyl and cyclopentadiene. Homogeneous catalysis by transition metal complexes, Catalytic steps, isomerisation, hydrogenation, hydroformylation and Ziegler-Natta polymerisation. Isolobal analogy in organometallic compounds. Synthesis and structure of organometallic compounds of Sn and Pb.

Unit 4: INORGANIC CHEMISTRY PRACTICAL (2 Credit)

Inorganic Quantitative Analysis:

Estimation of inorganic ions by volumetric, complexometric, gravimetric, redox and precipitation methods.

Separation and estimation of individual ions in two component systems of (a) Cu and Fe (b) Fe and Ca (c) Ca and Mg and (d) Cu and Ni.

(Any one of the above mixtures will be given for estimation in the examination.)

Semester VI

Paper: CHM601C (Molecular Spectroscopy)

Credit: 3+0+0 = 3

Unit 1: PRINCIPLES OF SPECTROSCOPY

10 L

The nature of electromagnetic radiation. The regions of the spectrum. Mechanism of interaction of electromagnetic radiation with matter. Absorption and emission spectroscopy, basic ideas of practical spectroscopy. Representation of spectrum, the width of spectral lines, selection rules for various transitions, intensity of spectral lines.

The Beer-Lambert law, molar decimal absorption coefficient and absorbance.

Unit 2: ROTATIONAL, VIBRATIONAL AND RAMAN SPECTROSCOPY

15 L

Rotational spectra of diatomic molecules – rigid rotor approximation. Determination of bond length, effect of isotopic substitution, spectra of non-rigid rotor. Vibrational spectra of diatomic molecules – harmonic and anharmonic oscillator model, Morse potential. Calculation of force constants, effect of isotopic substitution on vibrational frequency.

Vibrations of polyatomic molecules: normal modes of vibration (in H₂O, CO₂), overtone and combination bands (in H₂O, CO₂), Fermi resonance, hot bands.

Diatomic vibrating rotor, vibration-rotation spectrum of CO.

Principle of Raman Spectroscopy: rotational and vibrational Raman spectra of linear molecules. Selection rules for infrared and Raman spectra, rule of mutual exclusion.

Structure elucidation by infrared spectroscopy – stretching frequencies of bonds and functional groups (examples from both organic and inorganic molecules), concept of finger-print region. Correlation of infrared spectra with molecular structure – effects of conjugation, hydrogen bonding and coordination to metals on IR spectra.

Unit 3: ELECTRONIC SPECTROSCOPY

9 L

Selection rules for electronic transitions. Electronic transition in diatomic molecules: selection rules, Born-Oppenheimer approximation, vibrational structure, Franck-Condon principle, electronic transitions in polyatomic molecules.

Structure elucidation by UV-visible spectroscopy: chromophores (conjugated systems, carbonyl compounds), auxochrome, absorption due to ethylenic chromophore – Woodward's rule. Effect of solvents on electronic transition, quantitative estimations by spectrophotometry.

Introduction to photoelectron spectroscopy: UV-PES and XPS, chemical shift, Koopmann theorem.

Unit 4: SPIN RESONANCE SPECTROSCOPY

10 L

Interaction between spin and the magnetic field, nuclear spin, nuclear magnetic resonance spectroscopy, ¹H NMR spectroscopy. Presentation of the spectrum – chemical shift and its unit, approximate chemical shifts for simple organic molecules (alkanes, alkenes, alkynes, arenes, aldehydes, carboxylic acids and esters).

Spin-spin coupling and high resolution ^1H NMR spectrum of some simple organic molecules.

Basic concept of electron spin resonance (ESR) spectroscopy: Presentation of the spectrum, hyperfine structure, ESR of a few simple inorganic and organic ions and radicals.

Unit 5: MASS SPECTROSCOPY

4 L

Mass spectrometry: principles, idea of mass spectrometer. Simple applications in structure elucidation (alkane, aromatic hydrocarbon, primary alcohol, carbonyl compounds), Mc Lafferty rearrangement.

Paper: CHM602C (Organic Chemistry VI)

Credit: 3+0+1 = 4

Unit 1: ORGANIC PHOTOCHEMISTRY

14 L

Theory of photochemistry: Photophysical processes, electronic excitation and excited states. Law of photochemical equivalence, quantum yield, fluorescence and phosphorescence, Jablonski diagram, Franck-Condon principle. Quenching and photosensitizers.

Typical photochemical reactions: Photo-reduction of benzophenone, photolysis of ketones, Norrish type-I and Norrish type-II reactions, photo-isomerisation, dimerisation and cycloaddition of ethene.

Unit 2: CLASSES OF ORGANIC COMPOUNDS – IX

14 L

Active methylene compounds: The active methylene group. Synthesis of compounds containing active methylene groups (Ethylacetoacetate, diethylmalonate and ethyl cyanoacetate) and their use in organic synthesis.

Heterocyclic compounds: IUPAC nomenclature. Synthesis, structure, bonding, properties (basicity, aromaticity) and reactions of the following heterocycles: Furan, pyrrole, indole, thiophene, pyridine, quinoline and isoquinoline.

Unit 3: NATURAL PRODUCTS AND MEDICINAL CHEMISTRY

20L

Terpenes: Definition, isolation and classification, isoprene rule. Structure determination and synthesis of citral.

Alkaloids: Occurrence, general structural features, classification and properties. Structure and synthesis of nicotine.

Drugs: Basic classification. Analgesics: paracetamol and aspirin, their structure and preparation. Antibiotics: general idea including classification and structural variation. Sulpha drugs: general idea, mechanism of action, structure and preparation of sulphanilamide.

Unit 5: ORGANIC CHEMISTRY PRACTICAL

(1 Credit)

Organic Preparation

(a) Halogenation: Preparation of p-bromo acetanilide from acetanilide,

Preparation of 2,4,6-tribromophenol from phenol

(b) Oxidation: Preparation of benzil from benzoin.

(c) Reduction: Preparation of m-nitro aniline from m-dinitrobenzene
Students should recrystallise the prepared product and determine the melting point. Spectroscopic analyses (IR, UV-vis) of a few compounds prepared may be done.

Paper: CHM603C (Inorganic Chemistry VI) Credit: 3+0+2 = 5

Unit 1: ELECTRONIC SPECTRA OF COORDINATION COMPOUNDS 16L

Free ion terms and their splitting in octahedral symmetry, Orgel diagram, application of Tanabe-Sugano diagram. Laporte selection rule, vibronic coupling and colour of complexes, Electronic spectra of $M(H_2O)_6^{n+}$ complex ions. Effect of Jahn-Teller distortion on electronic spectra of coordination compounds. Charge-transfer spectra.

Unit 2: REACTIONS AND MECHANISMS IN COORDINATION CHEMISTRY 14L

Thermodynamic stability, stepwise formation constants, the chelate effect, kinetic lability and inertness: labile and inert compounds, mechanism of ligand displacement reactions in octahedral and square planar complexes, the trans effect, inner and outer sphere reactions.

Principles of colorimetric determination of metals. Determination of formation constants of complexes, Determination of composition of ionic compounds by conductometry, Theory of redox and complexometric titrations.

Unit 3: TRANSITIONAL AND INNER TRANSITIONAL ELEMENTS 10 L

Transitional elements: Electronic configuration and general periodic trends, comparative study of first transition series elements.

Trends in physical and chemical properties of second and third transition series in comparison to the first.

Lanthanides and Actinides: Electronic configuration, stability of oxidation states, lanthanide contraction, separation of the lanthanides, magnetic properties. Comparison of actinides with lanthanides, coordination compounds, colour and spectra.

Unit 4: NANOMATERIALS AND NANO SCIENCE 10 L

Fundamentals, novel optical properties of nanomaterials, characterisation and fabrication, self-assembled nanostructures. Control of nano-architectures: 1-D, 2-D and 3-D control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials: DNA and materials, natural and artificial nanomaterials. Bionanocomposites.

Unit 4: PROJECT / ADVANCED CHEMISTRY PRACTICAL (2 Credit)

EITHER,

A project work on a topic in any branch of Chemistry (Organic/ Inorganic/Physical/Theoretical Chemistry) including a brief review of the existing research literature on the same topic

OR,

Any one of the following sets of experiments may be done:

A. Detection of heavy metal content (As, Pb, Zn, Cu, Cd, Fe, Se, Cr, Ni, V etc.) in soil and water by using Atomic Absorption Spectrophotometer.

B. Inorganic Preparation – preparation of the following compounds:

1. Cu(glycinate)₂
2. Potassium trioxalato ferrate(III)
3. Cu(thiourea) complex
4. Copper tetraacetate

Students should recrystallize the prepared product and verify the presence/absence of anions and cations, as are applicable, by qualitative analysis. Spectroscopic investigations (IR, UV-vis) and room-temperature magnetic moment measurement of a few prepared complexes may be done.

Suggested Books for Chemistry Core (Major) Course:

Inorganic Chemistry:

1. Basic Inorganic Chemistry by F.A. Cotton, G. Wilkinson, P.L. Gaus (John Wiley and Sons Ltd.)
2. Concise Inorganic Chemistry by J.D. Lee (John Wiley and Sons Ltd., Indian Edition)
3. Inorganic Chemistry by G.L. Meissler and D.A. Tarr (Pearson)
4. Shriver and Atkins's Inorganic Chemistry by P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong (Oxford University Press, Indian Edition)
5. Chemistry of Elements by N.N. Greenwood and A. Earnshaw (Butterworth Heinemann)
6. Inorganic Chemistry Principles of Structure and Reactivity by J. E. Huheey, E.A. Keiter, R.L. Keiter and O.K. Medhi (Pearson Education)
7. Oxford Chemistry Primers: (1) Magnetochemistry by A.F. Orchard (2) Supramolecular Chemistry by P.D. Beer, P.A. Gale and D.K. Smith (Oxford University Press)
8. Fundamental Concepts of Inorganic Chemistry (Part I, II & III) by Ashim K. Das (CBS Publishers and Distributors)
9. Advanced Inorganic Chemistry (Volume I & II) by Satya Prakash, G.D. Tuli, S.K. Basu and R.D. Madan (S. Chand)

Organic Chemistry:

1. Organic Chemistry by J. Clayden, N. Greevs and S. Warren (Oxford University Press)
2. Organic Chemistry by S.H. Pine (McGraw Hill)
3. Organic Chemistry (Volume I & II) by I.L. Finar (Pearson)
4. Advanced Organic Chemistry by J. March (Wiley)
5. Advanced General Organic Chemistry by S.K. Ghosh (NCBA)
6. Organic Chemistry by S.M. Mukherji, S.P. Singh and R.P. Kapoor (Wiley)
7. Reaction Mechanism in Organic Chemistry by S.M. Mukherjee and S.P. Singh (Macmillan)
8. Basic Organic Stereochemistry by E.L. Eliel (Wiley)
9. Stereochemistry of Organic Compounds by D. Nasipuri (New Age International)
10. Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar (New Age International)

Physical Chemistry:

1. Atkins's Physical Chemistry by P. Atkins and J.D. Paula (Oxford University Press)
2. Physical Chemistry by I.N. Levine (Tata McGraw Hill)
3. Physical Chemistry by G.W. Castellan (Addison-Wesley)
4. A Textbook of Physical Chemistry (Volume 1, 2, 3, 4 & 5) by K.L. Kapoor (MacMillan)
5. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)
6. Modern Electrochemistry (Volume 1 & 2A) by J.O. Bokris and A.K.N. Reddy (Kluwer Academic)
7. General Chemistry by D.D. Ebbing and S.D. Gammon (Houghton Mifflin)
8. Essentials of Physical Chemistry by A. Bahl, B.S. Bahl and G.D. Tuli (S. Chand)

Quantum Chemistry and Spectroscopy:

1. Quantum Chemistry by I.N. Levine (Prentice Hall)
2. Quantum Chemistry by D.A. McQuarrie (University Science Books)

3. Quantum Chemistry and Spectroscopy by B.K. Sen (Kalyani)
4. Fundamentals of Molecular Spectroscopy by C.N. Banwell and E.M. McCash (Tata McGraw Hill)
5. Organic Spectroscopy by W. Kemp (MacMillan)
6. Vibrational Spectroscopy: Theory And Applications by D. N. Sathyanarayana (New Age International)
7. Introductory Organic Spectroscopy by B.K. Sen and Mousumi Ganguly (Kalyani)
8. Oxford Chemistry Primers: (1) Molecular Spectroscopy by J.M. Brown (2) NMR: The Toolkit by P.J. Hore, J.A. Jones and S. Wimperis (Oxford University Press)

Practical and Analytical Chemistry:

1. Vogel's Textbook of Practical Organic Chemistry edited by B.S. Furniss (Pearson)
2. Vogel's Textbook of Quantitative Inorganic Analysis (Longman)
3. Vogel's Textbook of Qualitative Inorganic Analysis, revised by G. Svehla (Pearson)
4. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra (New Central Book Agency)
5. Advanced Practical Inorganic Chemistry by Gurdeep Raj (Goel Publishing)
6. Advanced Practical Organic Chemistry by O.P. Agarwal (Goel Publishing)
7. Advanced Practical Physical Chemistry by J.B. Yadav (Krishna Prakashan Media)
8. Analytical Chemistry by G.D. Christian (John Wiley)
9. Applications of Absorption Spectroscopy of Organic Compounds by J.R. Dyer (Prentice-Hall)
10. Infrared and Raman Spectra of Inorganic and Coordination Compounds by K. Nakamoto (Wiley)

COTTON COLLEGE STATE UNIVERSITY

Guwahati, Assam

DRAFT SYLLABUS

DEGREE COURSE (B.Sc.) SYLLABUS IN CHEMISTRY

ELECTIVE COURSE

Semester I

Paper: CHM104E (Elective Chemistry I) Credit: 3+0+0 = 3

Unit 1: ATOMIC STRUCTURE 14L

Origin of quantum theory: photoelectric effect, quantisation of energy – atomic line spectra of hydrogen, dual nature of matter (de Broglie relation), Heisenberg's uncertainty principle. Schrodinger's time-dependent and time-independent equation, physical interpretation of the wave function.

Solution of Schrodinger equation for the electron of H-atom (qualitative idea only), quantum numbers, orbital wavefunction, radial function and angular function, plots of radial function (qualitative idea only) for 1s, 2s, 2p, 3s, 3p, 3d subshells.

Many electron atoms: Effective nuclear charge, screening and penetration effects, energy ranking of the 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p etc. subshells. Electron spin and spin quantum number. Electronic configuration of atoms, Aufbau principle, Pauli's principle, Hund's rule.

Unit 2: COVALENT BONDING 14L

Valence bond approach : Lewis electron pair bonds (in H_2 , HF, O_2 , N_2 , NH_3 , H_2O , H_2O_2). Shapes of molecules – principle and applications of valence shell electron pair repulsion (VSEPR) theory (as in BF_3 , CH_4 , NH_3 , H_2O , PCl_5 , SF_6). Hybridisation (as in BeH_2 , C_2H_2 , C_2H_4 , CH_4 , BF_3 , CO_3^{2-} , PCl_5 , SF_6 and C_6H_6). Resonance (as in C_6H_6 , O_3 , CO_3^{2-} , NO_3^-), resonance energy, delocalisation in benzene.

Polar molecules – the concept of electronegativity (Pauling and Mulliken scale). Dipole moment and bond moment (as in CO_2 , H_2O , NH_3 , NF_3). Percentage ionic character of bonds (as in HF, HCl, HBr).

Unit 3: STATES OF MATTER 20L

Gases: Distribution of molecular speed – Maxwell's speed distribution law (no derivation). Concept of mean, root mean square (r.m.s.) and most probable speeds – their expressions from the speed distribution law. Kinetic theory of gases: Postulates, expression of pressure in terms of the r.m.s. speed of gas molecules (no derivation), relation with average molecular kinetic energy. Degrees of freedom, principle of equipartition of energy. Deviation from ideal behaviour, van der Waals equation of state and its explanation, critical phenomena and critical constants, derivation of expressions of critical constants from van der Waals equation.

Liquids: Properties of liquids, definition and experimental measurement of vapour pressure (dynamic method), surface tension (drop number method) and coefficient of viscosity (Ostwald method). Variation of these properties with temperature.

Solids: Crystal lattices, unit cells, the seven crystal systems and fourteen Bravais lattices. Density and packing fraction in simple cubic, fcc and bcc lattices. Closed packed structures. Imperfections in solids: point defects, introduction to Schottky and Frenkel defects.

Semester II

Paper: CHM204E (Elective Chemistry II)

Credit: 2+0+1 = 3

Unit 1: ORGANIC COMPOUNDS – I

18L

Introduction to classification and IUPAC nomenclature of organic compounds, for the following classes:

(a) Alkanes: Preparation (Wurtz, Kolbe, Corey-House reactions), their properties and reactions. Homolytic bond fission, free radical generation and reactivity – photo-chemical chlorination of alkanes.

(b) Cycloalkanes: Bayer's strain theory. Angle strain, banana bond in cyclopropane ring. Shapes of cyclohexane rings, conformations of cyclohexane.

(c) Alkenes : Preparation (elimination of alkyl halides, alcohols), Wittig reaction, pyrolysis of esters. Reactions of alkenes. diastereomerism, stability and interconversion. Markownikov and Saytzeff rules, mechanism of electrophilic addition reaction.

(d) Alkynes and alkadienes: Preparation, properties, reactions of alkynes. Addition reactions of alkynes with polar reagents, ozonolysis, catalytic hydrogenation (Lindlar's catalyst). Structures and industrial significance of 1,3-butadiene and isoprene. Basic ideas of pericyclic reactions shown by conjugated dienes such as 1,3-butadiene.

(e) Arenes: Aromaticity. Preparation and reactions of benzene. Mechanism of electrophilic aromatic substitution. Activation, deactivation and directive influence of groups. Conversion of benzene to its derivatives and vice versa. Polynuclear aromatic hydrocarbons (PAH): structure, preparation and reactions (electrophilic substitution reactions) of naphthalene and anthracene, significance of PAH-s as carcinogens.

Unit 2: CHEMICAL KINETICS

14L

Reaction rates and rate laws. Order and molecularity of a reaction. Differential and integrated rate equation of first and second order reactions of type $A \rightarrow P$ only. Experimental determination of reaction rates.

Simple consecutive reactions and chain reactions: steady state approximation (SSA) and the rate determining step (RDS) approximation – application in decomposition of dinitrogen pentoxide and thermal decomposition of ethanal.

Effect of temperature on reaction rate – the Arrhenius equation. Collision theory of reaction rates (qualitative treatment only).

Homogeneous catalysis: oxidation of SO_2 to SO_3 catalysed by NO, acid-base catalysis (as in hydrolysis of methyl ethanoate), enzyme catalysis – Michaelis-Menten equation.

Unit 3: CHEMISTRY PRACTICAL

(1 Credit)

Qualitative organic analysis:

a) Detection of N, S and halogens in organic compounds.

b) Detection of functional groups (one among the following):

–OH (phenolic), C=O (ketone), –COOH, –NH₂, –NO₂

(At least five organic compounds need be analysed during the session)

Semester III

Paper: CHM304E (Elective Chemistry III)

Credit: 2+0+1 = 3

Unit 1: CHEMICAL THERMODYNAMICS

14L

Basic definitions and concepts: system, surroundings, process, state function, path function, heat transferred, work done. The first law of thermodynamics: concept of internal energy, mathematical forms of first law for infinitesimal and finite processes in a system. Definition of enthalpy and its significance. Definition and concept of between C_p and C_v : their general inter-relation, inter-relation for an ideal gas.

Thermochemistry – enthalpy of reaction, relation between ΔH and ΔU . Standard enthalpy changes. Hess's law and Kirchhoff's law.

The second law of thermodynamics. Relation between entropy and spontaneity of processes, calculation of entropy changes during vapourisation and fusion. Gibbs free energy and its significance. Free energy change and spontaneity. Thermodynamic criteria for chemical equilibrium; the relation between standard free energy change and the equilibrium constant.

Unit 2: INTERMOLECULAR FORCES AND IONIC BONDING

8L

Intermolecular forces: dispersion forces, dipole-dipole and ion-dipole interactions, hydrogen bonds, ionic bonds, influence of hydrogen bonds on water and ice.

Properties of ionic solids, Lattice energy of ionic compounds and its calculation using Born-Haber cycle as in NaCl. Partial covalency in ionic compounds – Fajan's rule of polarisation. Consequences of polarisation on melting points, boiling points and solubility of ionic solids.

Unit 3: REACTIVE INTERMEDIATES AND STEREOCHEMISTRY

10L

Reactive intermediates: carbocations and carbanions – their shape, generation, stability and reactions.

Stereochemistry: Classification – geometrical isomers (simple examples involving alkenes, cis-trans and E-Z nomenclature), optical isomers (concepts of chirality, enantiomers and diastereomers, meso structures, racemic mixtures, D-L and R-S notations) and conformational isomers (eclipsed and staggered conformations of ethane with their Newman projections).

Unit 4: GENERAL CHEMISTRY EXPERIMENTS

(1 Credit)

- To determine the water of crystallization of green vitriol by titration of its prepared solution with KMnO_4 solution.
- To determine the solubility of a salt at room temperature.
- To determine the coefficient of viscosity of a given aqueous solution using an Ostwald viscometer.
- To determine the surface tension of a given aqueous solution by using a stalagmometer.

Semester IV

Paper: CHM404E (Elective Chemistry II)

Credit: 2+0+1 = 3

Unit 1: CHEMISTRY OF NON-TRANSITION ELEMENTS

14L

Group-wise study of physical properties, chemical reactivity of elements and their important compounds – oxides and hydroxides, oxyacids, halides, hydrides (for the groups 1, 15, 16, 17).

Periodicity: General trends in size, ionisation energy, electron affinity and electronegativity, first and second row anomalies, diagonal relationships, the use of d-orbitals by third period elements, catenation and inert pair effect (in Pb and Tl).

Inorganic chains, rings and cages: Synthesis, structure and reactions of silicones, borazine and diborane.

Carbides and nitrides. Interhalogen compounds, polyhalides, pseudohalogens – synthesis and structure. Noble gas compounds: synthesis, structure and bonding.

Unit 2: ORGANIC COMPOUNDS – II

18L

Alkyl halides and 1,2-dihalides: Preparation, properties and reactions of alkyl halides. Mechanism of S_N1 and S_N2 reactions, E_1 and E_2 reactions. Effect of solvent, substrate and other factors on the mechanism. Substitution vs elimination. Conversion of alkyl halides to alcohols, ethers, amines and nitriles. Preparation and synthetic uses of Grignard reagent.

Alcohols: Classification of alcohols, 1°, 2°, 3° alcohols and their distinguishing reactions, glycols and glycerol, IUPAC nomenclature. General methods of preparation, properties and general reactions of primary alcohols, glycols and glycerol. Basic concept of hydrogen bonding and their influence on properties of organic compounds. Benzyl alcohol – preparation and reactions.

Ethers: Williamson's ether synthesis and hydrolysis of ethers.

Phenols: Synthesis and reactions of phenols. Acidity of phenols and substituted phenols. Electrophilic aromatic substitution of phenols. Use of phenol in synthesis of Bakelite.

Amines: 1°, 2°, 3° amines. Basicity of amines. Preparation, properties and reactions of 1° amines. Synthesis, properties and reactions of aniline. Basicity of aniline and substituted aniline. Electrophilic aromatic substitution. Diazonium ions and their synthetic utility.

Unit 3: CHEMISTRY PRACTICAL

(1 Credit)

Qualitative inorganic analysis:

Identification of the following in an inorganic salt:

Cations: Hg^{2+} , Pb^{2+} , Cu^{2+} , Bi^{3+} , As^{3+} , Sb^{3+} , Sn^{2+}/Sn^{4+} , Fe^{2+}/Fe^{3+} , Cr^{3+} , Al^{3+} ,
 Co^{2+} , Ni^{2+} , Mn^{2+} , Zn^{2+} , Ba^{2+} , Ca^{2+} , Sr^{2+} , Mg^{2+}

Anions: Cl^- , Br^- , I^- , NO_2^- , NO_3^- , S^{2-} , SO_3^{2-} (without interfering radicals)

(Presence of Na^+ , K^+ , NH_4^+ and CO_3^{2-} radicals are to be ignored and not to be reported. At least four salts must be analysed during the session.)

Semester V

Paper: CHM504E (Elective Chemistry V)

Credit: 2+0+1 = 3

Unit 1: CHEMISTRY OF TRANSITION ELEMENTS

10L

Comparative study of elements of first transition series with emphasis on electronic configuration, relative stability of oxidation states, ionisation potentials, redox potentials, reactivity.

Occurrence, principles of extraction of Cr, Mn and Ni and their important compounds (e.g., KMnO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$).

Werner theory, types of ligands, Isomerism and IUPAC nomenclature of coordination complexes. Chelates.

Essential and trace elements useful to life: introduction to their biological role. Toxicity due to metals and non-metals. Use of metal compounds in medicine.

Unit 2: INTRODUCTION TO BIOCHEMISTRY

12L

Amino acids and peptides: Elementary ideas of amino acids, essential amino acids, optical activity, D-L nomenclature, peptides and proteins. Synthesis and reaction of glycine. Simple methods of preparation of dipeptides. Concept of primary and secondary structure in proteins.

Carbohydrates: Open chain and ring structure of glucose and fructose. Concept of mutarotation, anomers, epimers. Reaction of glucose and fructose. Structure of ribose and deoxyribose sugars. Structure of sucrose, starch and cellulose.

Lipids: Structure and physical properties of saturated fats and unsaturated fats (oils). Structure and general preparation of soaps. Analysis of fats and oils.

Nucleic acids: general idea, the double helical structure of RNA and DNA, meaning of nucleotide and nucleoside units. The sugar, nucleobase and phosphate components. The purine and pyrimidine nucleobases. Concept of complimentary bases, gene and the expression of genetic code in terms of arrangement of nucleobases.

Unit 3: SURFACE CHEMISTRY

10L

Physisorption and chemisorption. Freundlich, Langmuir and BET adsorption isotherms (derivations not required), their validity and significance. Heterogeneous catalysis – adsorption theory (qualitative treatment only).

Surfactants – Definition, explanation of surface tension lowering and cleansing actions. Micelle formation and critical micelle concentration.

Colloids – Classification, preparation and purification, structure and stability.

Unit 4: CHEMISTRY PRACTICAL

(1 Credit)

Qualitative inorganic analysis:

Identification of not more than three radicals in a mixture of the following, including interfering anionic radicals:

Cations: Hg^{2+} , Pb^{2+} , Cu^{2+} , Bi^{3+} , As^{3+} , Sb^{3+} , $\text{Sn}^{2+}/\text{Sn}^{4+}$, $\text{Fe}^{2+}/\text{Fe}^{3+}$, Cr^{3+} , Al^{3+} ,
 Co^{2+} , Ni^{2+} , Mn^{2+} , Zn^{2+} , Ba^{2+} , Ca^{2+} , Sr^{2+} , Mg^{2+}

Anions: Cl^- , Br^- , I^- , NO_2^- , NO_3^- , S^{2-} , SO_3^{2-} , F^- , BO_3^{3-} , PO_4^{3-}

(Presence of Na^+ , K^+ , NH_4^+ and CO_3^{2-} radicals are to be ignored and not to be reported.

At least four salt mixtures must be analysed during the session.)

Semester VI

Paper: CHM604E (Elective Chemistry VI)

Credit: 2+0+1 = 3

Unit 1: PHASE EQUILIBRIUM

6L

Definition of phases, components and degrees of freedom. Gibbs Phase rule. Phase diagram of the water system. Binary liquid-liquid solutions: Raoult's law, ideal and non-ideal solutions, distillation behaviour for positive and negative deviations, azeotropes (as in water-ethanol, water-HCl systems).

Unit 2: ION TRANSPORT AND ELECTROCHEMISTRY

16L

Conductance of electrolytes – conductance, conductivity and molar conductivity. Measurement of conductance and application of conductance measurements. Conductometric titrations. Variation of molar conductivity with concentration. Kohlrausch's law of independent migration of ions. Transport number of ions and their determination.

Galvanic cells – definition, description and working processes. Standard electrode potentials and electromotive force (emf). The Nernst equation and calculation of cell potential. Concentration cells. Relation between cells emf and equilibrium constant. Standard and reference electrodes. Measurement of pH. Commercial applications of galvanic cells – dry cell, lead storage battery, fuel cells.

Dissociation equilibria of weak electrolytes, Ostwald's dilution law, the pH scale, strengths of acids and bases – expression in terms of pK_a and pK_b . Solubility products and its application in analytical chemistry. Henderson-Hasselbach equation and calculation of pK_a values. Buffer solutions and buffer action, uses of buffer solutions in chemistry and biology.

Unit 3: CARBONYL COMPOUNDS AND CARBOXYLIC ACIDS

10L

General methods of preparation and reactions of carbonyl compounds (methanal, ethanal, propanone and 2-butanone as examples). Difference in reactivity of aldehydes and ketones. Polarization of carbonyl group. Nucleophilic addition of aldehydes and ketones.

Carboxylic acids: preparation, influence of substituents on acidity of carboxylic acids. General reactions of aliphatic and aromatic carboxylic acids (methanoic, ethanoic and benzoic acids). Conversion of carboxylic acids to their derivatives.

Unit 4: CHEMISTRY PRACTICAL

(1 Credit)

Estimation by volumetric method of the following:

- Fe(II) – by using $KMnO_4$ solution (standardisation of the $KMnO_4$ solution using oxalic acid solution need to be performed by each student).
- Fe(III) – by using $K_2Cr_2O_7$ solution (the standard $K_2Cr_2O_7$ solution need to be prepared by each student).
- The total hardness of water – by titration with EDTA.

Suggested Books:

1. General Chemistry by D.D. Ebbing and S.D. Gammon (Houghton Mifflin)
2. Concise Inorganic Chemistry by J.D. Lee (John Wiley and Sons Ltd., Indian Edition)
3. Organic Chemistry by S.M. Mukherji, S.P. Singh and R.P. Kapoor (Wiley)
4. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)
5. Vogel's Textbook of Qualitative Inorganic Analysis, revised by G. Svehla (Pearson)
6. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra (New Central Book Agency)