Cotton College State University
Department of Chemistry
Undergraduate Syllabus

Paper Code	Paper Title	L+T+P	Credits
SEMESTER I			
CHM 101C	Physical Chemistry I	3+0+1	4
CHM 102C	Organic Chemistry I	3+0+1	4
CHM 103C	Inorganic Chemistry I	3+0+1	4
CHM 104E	Chemistry I	3+0+0	3
SEMESTER II			
CHM 201C	Physical Chemistry II	3+0+1	4
CHM 202C	Organic Chemistry II	3+0+2	5
CHM 203C	Inorganic Chemistry II	3+0+0	3
CHM 204E	Chemistry II	2+0+1	3
SEMESTER III			
CHM 301C	Physical Chemistry III	3+0+0	3
CHM 302C	Organic Chemistry III	3+0+0	3
CHM 303C	Inorganic Chemistry III	3+0+3	6
CHM 304E	Chemistry III	2+0+1	3
SEMESTER IV			
CHM 401C	Physical Chemistry IV	3+0+2	5
CHM 402C	Organic Chemistry IV	3+0+0	3
CHM 403C	Inorganic Chemistry IV	3+0+1	4
CHM 404E	Chemistry IV	2+0+1	3
SEMESTER V			
CHM 501C	Quantum Chemistry	3+0+0	3
CHM 502C	Organic Chemistry V	3+0+1	4
CHM 503C	Inorganic Chemistry V	3+0+2	5
CHM 504E	Chemistry V	2+0+1	3
SEMESTER VI			
CHM601C	Molecular Spectroscopy	3+0+0	3
CHM602C	Organic Chemistry VI	3+0+1	4
CHM603C	Inorganic Chemistry VI	3+0+2	5
CHM604E	Chemistry VI	2+0+1	3

SEMESTER I

CHM 101C	**Physical Chemistry I**	**3+0+1**	**4**
CHM 102C	**Organic Chemistry I**	**3+0+1**	**4**
CHM 103C	**Inorganic Chemistry I**	**3+0+1**	**4**
CHM 104E	**Chemistry I**	**3+0+0**	**3**

CHM 101C: (Physical Chemistry I)
No of lectures – 48

Course outline—

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: CHEMICAL THERMODYNAMICS – II 16L

The unidirectional nature of spontaneous processes, the zeroth law of thermodynamics. 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., $G = \Sigma_i n_i \mu_i$), the Gibbs-Duhem equation and its derivation.

The Nernst heat theorem and third law of thermodynamics.

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, H_2-Br_2 reaction, thermal decomposition of ethanal, branching and non-branching chain reaction, H_2-O_2 reaction, concept of explosion limits.

Introduction to polymerisation kinetics of free-radical chain polymerisation.

Unit 4: PHYSICAL CHEMISTRY PRACTICAL (1 Credit)

(a) Determination of the concentrations of sodium carbonate and sodium hydroxide in a mixture of the two in aqueous solution.

(b) To determine the solubility of a given substance at different temperatures and to plot the solubility curve.

(c) Determination of equivalent mass of an acid (e.g., oxalic acid) by direct titration method.

CHM 102C: (Organic Chemistry I)

No of lectures – 48

Course outline—

Unit 1: INTRODUCTION TO ORGANIC COMPOUNDS 10 L

Classification of organic compounds on the basis of their functional groups, homologous series. IUPAC nomenclature for organic compounds with single and multiple functional groups. Chain, position and functional group isomerism. Special types of compounds e.g., 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. 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 12L

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 disymetry, asymmetry, enantiomers and diastereomers, racemic mixtures, resolution of racemic mixtures.

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

Unit 4: ORGANIC REACTION MECHANISMS – I 16L

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. IUPAC nomenclature system for organic transformations. 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 mechanism. Elimination reaction: β–elimination reaction - base catalysed and pyrolytic elimination.

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: Preparation of acetanilide from aniline OR preparation of aspirin from salicylic acid (any one only).
   (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.

CHM 103C: (Inorganic Chemistry I)

No of lectures – 48

Course outline—

Unit 1: FUNDAMENTALS OF ATOMIC STRUCTURE 16L

Outlines of some quantum-mechanical ideas regarding atomic structure:

(a) Discrete nature of energy levels of atomic and molecular systems, Line spectra of atoms: hydrogen atom spectra and its various series. Band spectra of molecules.

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

(c) 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.

(d) 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).

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

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

(g) Effective nuclear charge – shielding and penetration effects. 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 H_2).

Resonance and resonance energy in HF and benzene.

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

Percent ionic character of HCI 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, NO_2). Multiple bonding, orbital picture and energy levels of ethane, ethyne and benzene, Huckel's aromaticity rule. Delocalisation vs. Resonance. 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.

CHM 104E: (Chemistry I)
No of lectures – 48

Course outline—

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

CHM 201C	**Physical Chemistry II**	**3+0+1**	**4**
CHM 202C	**Organic Chemistry II**	**3+0+2**	**5**
CHM 203C	**Inorganic Chemistry II**	**3+0+0**	**3**
CHM 204E	**Chemistry II**	**2+0+1**	**3**

CHM 201C: (Physical Chemistry II)
No of lectures – 48

Course outline—

Unit 1. THE GASEOUS STATE OF MATTER 13L

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.

Transport properties of gases, concept of flux and the Fick's law of diffusion. Rate of diffusion, thermal conductivity and coefficient of viscosity of a gas from kinetic theory.

Unit 2: LIQUIDS AND COLLOIDS 13L

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 3: COLLIGATIVE PROPERTIES 10L

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 4: ELECTROCHEMISTRY – I 12L

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 5: PHYSICAL CHEMISTRY PRACTICAL (1 Credit)

(a) To determine the concentration of an optically active substance and also its specific rotation by polarimetric measurements.
(b) Conductometric titration of aq. HCl vs. aq. NaOH.
(c) pH-metric titration of aq. CH_3COOH vs. aq. NaOH.

CHM 202C: (Organic Chemistry II)
No of lectures – 48

Course outline—

Unit 1: ORGANIC REACTION MECHANISMS – II 13 L

Substitution reactions: electrophilic and nucleophilic. Nucleophilic aliphatic substitution – S_N1 and S_N2 reactions.and free radical mechanism

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

b) Mechanism of nucleophilic aromatic substitution. Intermediate complex mechanism, benzyne mechanism. Directive influences in benzyne mechanism. Cine substitution, methods of trapping benzyne intermediates.

Unit 3: 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 2: CLASSES OF ORGANIC COMPOUNDS – II 9 L

Alkyl haildes: Preparation and reactions. Elimination vs. substitution reactions – controlling factors.

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

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

Unit 4: CLASSES OF ORGANIC COMPOUNDS – III 16 L

Alkenes: Preparation of alkenes with special reference to dehydrohalogenation and to dehydration of alcohols. Mechanism of elimination reactions: Saytzeff and Hoffmann elimination. Properties of alkenes with special emphasis on addition to C=C bond. Mechanism of electrophilic addition, Markownikoff's rule. Free radical addition to alkenes. Peroxide effect. Hydroboration, oxymercuration-demercuration, epoxidation, 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:

(a) Detection of nitrogen, sulphur and halogens.

(b) Test for functional groups by analytical methods.

(c) Solubility and melting point/ boiling point

(d) Preparation of a derivative and determination of its melting point.

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

CHM 203C: (Inorganic Chemistry II)
No of lectures – 48

Course outline—

Unit 1: 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):

(a) Electronic configuration, effective nuclear charge, Slater's rule, size of atoms, ions and atomic orbitals.

(b) Ionisation energy and electron affinity of atoms.

(c) Tendency to use vacant d-orbitals and electropositive character of metals.

(d) 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.

(e) Melting point and boiling point of elements and their compounds.

(f) Solubility of salts and molecules in water.

(g) 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.

(h) Catenation and inert-pair effect.

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

Unit 2: 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:

(a) Ortho and para hydrogen, hydrates, clathrates and inclusion compounds, binary metallic hydrides.

(b) Allotropes of carbon (including fullerenes), graphite, intercalation compounds, carbides, cyanogens, oxides and oxy-acids of carbon.

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 N_2O

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, S_4N_4, P_4, P_4O_6, P_4O_{10}, diborane, boron cage compounds, carboranes and metallocarboranes.

CHM 204E: (Chemistry II)
No of lectures – 32

Course outline—

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. π-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): structures of naphthalene and anthracene, significance of PAH-s as carcinogens found in some foods.

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 Arhenius 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, $-NH_2$

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

SEMESTER III

CHM 301C	**Physical Chemistry III**	**3+0+0**	**3**
CHM 302C	**Organic Chemistry III**	**3+0+0**	**3**
CHM 303C	**Inorganic Chemistry III**	**3+0+3**	**6**
CHM 304E	**Chemistry III**	**2+0+1**	**3**

CHM 301C: (Physical Chemistry III)
No of lectures – 48

Course outline—

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.

CHM 302C: (Organic Chemistry III)
No of lectures – 48

Course outline—

Unit 1: ORGANIC STEREOCHEMISTRY – II 9 L

Conformation of cyclohexane: boat and chair forms. Relative stability and torsional strain of the conformers of ethane, butane and cyclohexane.

Concept of topocity and prostereoisomerism. Criteria of establishing topocity 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, Cannizaro reaction, Claisen condensation, Reformatsky reaction, Oppeneauer reaction, Wolff-Kishner reduction, Benzoin condensation, Wittig reaction, Beckmann rearrangement, benzil-benzillic acid 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.

Unit 4: CLASSES OF ORGANIC COMPOUNDS – VI 10 L

Ethers: preparation, cleavage and auto-oxidation reactions. Epoxides: preparation, acid and base catalysed ring opening, orientation of ring-opening, reaction of Grignard and organolithium reagents.

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.

Organo-Sulphur Compounds: Preparation and reactions of thiols, thioethers and sulphonic acids.

CHM 303C: (Inorganic Chemistry III)
No of lectures – 48

Course outline—

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.

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

Symmetry of crystals, general features of diffraction (Bragg's law); Introduction to X-ray crystallography and determination of structure of solids.

Unit 3: TRANSITION METALS 18L

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.

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.

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)

CHM 304E: (Chemistry III)
No of lectures – 32

Course outline—

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)

(a) To determine the water of crystallization of green vitriol by titration of its prepared solution with $KMnO_4$ solution.

(b) To determine the solubility of a salt at room temperature.

(c) To determine the coefficient of viscosity of a given aqueous solution using an Ostwald viscometer.

(d) To determine the surface tension of a given aqueous solution by using a stalagmometer.

SEMESTER IV

CHM 401C	**Physical Chemistry IV**	**3+0+2**	**5**
CHM 402C	**Organic Chemistry IV**	**3+0+0**	**3**
CHM 403C	**Inorganic Chemistry IV**	**3+0+1**	**4**
CHM 404E	**Chemistry IV**	**2+0+1**	**3**

CHM 401C: (Physical Chemistry IV)
No of lectures – 48

Course outline—

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 H_2-Br_2, H_2-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 1: SURFACE CHEMISTRY AND CATALYSIS 12L

Introduction to solid surfaces, adsorption at surfaces – physisorption and chemisorption. Adsorption isotherms – Langmuir isotherm and its derivation. Determination of surface area, catalytic activity at surface with examples. Concept of surface excess, Gibbs equation, surface pressure and surface spreading.

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)

(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 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 $KMnO_4$/ $K_2Cr_2O_7$/ $CuSO_4$ using spectrophotometer.
(g) Determine the composition of iron(III)-thiocyanato complex spectrophotometrically by Job's method of continuous variation

CHM402C (Organic Chemistry IV)
No of lectures – 48

Course outline—

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 iodic acid, osmium tetroxide, mechanism of the oxidation reactions. Typical oxidation reactions – Oppenaeur oxidation.

Mechanism of reduction reactions occurring through:

(i) Direct electron transfer – e.g., Clemmensen reduction (Nakabayashi mechanism).
(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 18 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.

Nucleotides, nucleosides and nucleic acids: general idea, the sugar, nucleobase and phosphate components, definition of purine and pyrimidine bases. Gene and the genetic code in terms of arrangement of nucleobases.

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

Carbohydrates: general idea of monosaccharides, disaccharides and polysaccharides. Structures of ommon pentose and hexose monosaccharides.

Unit 3: INTRODUCTION TO GREEN CHEMISTRY 10 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.

CHM 403C: (Inorganic Chemistry IV)
No of lectures – 48

Course outline—

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: LANTHANIDES AND ACTINIDES 10 L

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 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

Physical properties of the proton and the neutron, structure of the nucleus, mass defect and binding energy. Radioactive decay and equilibrium. Nuclear reactions, Q value, nuclear cross sections.

Theory of radioactive disintegration, rates of disintegration, the radiochemical series. Transmutation of elements and artificial radioactivity, fission and fusion. Nuclear reactions and their use, methods of measurement of 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

Students should recrystallise the prepared product and verify the presence/ absence of anions and cations, as are applicable, by qualitative analysis.

CHM 404E: (Chemistry II)
No of lectures – 32

Course outline—

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, thioethers and thiols. 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 reaction.

Ethers: Willamson'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

CHM 501C	**Quantum Chemistry**	**3+0+0**	**3**
CHM 502C	**Organic Chemistry V**	**3+0+1**	**4**
CHM 503C	**Inorganic Chemistry V**	**3+0+2**	**5**
CHM 504E	**Chemistry V**	**2+0+1**	**3**

CHM 501C: (Quantum Chemistry)
No of lectures – 48

Course outline—

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.

CHM 502C: (Organic Chemistry V)
No of lectures – 48

Course outline—

Unit 1: MOLECULAR REARRANGEMENTS 10 L

(i) Nucleophilic or anionotropic: 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.

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 and isonitriles, and aromatic nitro compounds.

Organo-phosphorus compounds: Phosphines, phosphorus esters and phosphorus ylides – Wittig reaction.

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, 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.

Biopolymers: polysaccharides (cotton etc.) and polypeptides (wool etc.), structure of cellulose, starch and lignins.

Unit 4: BIOCHEMISTRY – II 10 L

Structure of RNA and DNA, Watson-Crick hydrogen bonds in DNA, Biosynthesis of DNA (replication), of RNA (transcription) and of proteins (translation).

Enzymes and their function as catalysts: Chymotripsin and lysozyme. Metalloenzymes and coenzymes.

Hormones: Definition, classification and basic functions.

Fundamentals of biological energy production: Glycolysis, Kreb's cycle. photosynthesis, respiration, oxidative phosphorylation and ATP synthesis.

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 – Cope and Claisen rearrangement.

Unit 6: ORGANIC CHEMISTRY PRACTICAL (1 Credit)

Organic quantitative analysis:

(a) Determination of equivalent mass of an acid by titrimetric method.

(b) Determination of amount of glucose by titration with Fehling's solution.

(c) Estimation of urea by hypobromite method.

CHM 503C: (Inorganic Chemistry V)
No of lectures – 48

Course outline—

Unit 1: 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 2: 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 3: BIOINORGANIC CHEMISTRY 16L

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 4: NANOMATERIALS AND NANO SCIENCE 10L

Fundamentals, novel optical properties of nanomaterials, charcterisation 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 5: INORGANIC CHEMISTRY PRACTICAL (2 Credit)

Inorganic Quantitative Analysis:

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

The following one-component systems should be estimated first: Cu, Fe, Ca, Mg, Ni, Cl^-, and SO_4^{2-}. This should be followed by separation and estimation of individual ions in two component systems of (a) Cu and Fe (b) Fe and Ca (c) Ca and Mg (d) Cu and Ni and (e) Cl^- and SO_4^{2-}

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

CHM 504E: (Chemistry V)
No of lectures – 32

Course outline—

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., $KMnO_4$, $K_2Cr_2O_7$).

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+}, 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-}, 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

CHM601C	**Molecular Spectroscopy**	**3+0+0**	**3**
CHM602C	**Organic Chemistry VI**	**3+0+1**	**4**
CHM603C	**Inorganic Chemistry VI**	**3+0+2**	**5**
CHM604E	**Chemistry VI**	**2+0+1**	**3**

CHM 601C: (Molecular Spectroscopy)
No of lectures – 48

Course outline—

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. Molecular motions and energy – degrees of freedom, moment of inertia.

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 H_2O, CO_2), overtone and combination bands (in H_2O, CO_2), 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 and its applications in chemistry.

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 ethanol, ethyl benzoate, 2-iodopropane and cyanohydrin.

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, fragmentation pattern. Simple applications in structure elucidation (butane, ethanol, acetone), Mc Lafferty rearrangement (hexanoic acid, pentanal), nitrogen rule.

CHM 602C: (Organic Chemistry VI)
No of lectures – 48

Course outline—

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

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.

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 few compounds prepared may be done.)

CHM 603C: (Inorganic Chemistry VI)
No of lectures – 48

Course outline—

Unit 1: ELECTRONIC SPECI'RA 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 liability 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: ORGANOMETALLIC COMPOUNDS 18L

Synthesis, structure and bonding of complexes with olefins, acetylene, allyl, cyclopentadiene and arenes. IUPAC nomenclature. Effective atomic number rule, Transition metal to carbon sigma bonds. Isolobal analogy in organometallic compounds, Carbonyl and binuclear carbonyl complexes.

Homogeneous catalysis by transition metal complexes (isomerisation, hydrogenation, hydroformylation and Ziegler-Natta polymerisation).

Synthesis and structure of organometallic compounds of Sn and Pb. Organometallic compounds of Zn, Cd and Hg.

Unit 4: INORGANIC CHEMISTRY PRACTICAL (2 Credit)

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. Potassium trioxalato chromate(III)
4. Cu(thiourea) complex
5. 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.)

CHM 604E: (Chemistry VI)
No of lectures – 32

Course outline—

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, desciption 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 ketons, mechanism with examples. Preparation and reactions of benzaldehyde and acetophenone.

Acidity of carboxylic acids, and substituted carboxylic acids. General methods of
preparation, properties and reactions of aliphatic carboxylic acid (methanoic, ethanoic and propanioc acid as examples). Synthesis , properties and reactions of benzoic acid. Acidity of substituted benzoic acids. Conversion of carboxylic acids to their derivatives. Synthetic uses of ethylacetoacetate and diethylmalonate.

Unit 4: CHEMISTRY PRACTICAL (1 Credit)

Estimation by volumetric method of the following:

(a) Fe(II) – by using $KMnO_4$ solution (standardisation of the $KMnO_4$ solution using oxalic acid solution need to be performed by each student).
(b) Fe(III) – by using $K_2Cr_2O_7$ solution (the standard $K_2Cr_2O_7$ solution need to prepared by each student).
(c) 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)

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. Overtone, J. Rourke, M. Weller and F. Armstrong (Oxford University Press, Indian Edition)
5. Chemistry of Elements by N. N. Greenwood and A. Earnshow (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)