U.G. 2nd Semester

Paper: CHM201C (Core)
Organic Chemistry I

Credits: 5 = 3+0+2 (45 Lectures)

Theory: 45 Lectures

Unit 1: Recapitulation of Basics of Organic Chemistry (6 Lectures)

Hybridization, Shapes of molecules

Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and its applications, Dipole moment; Hydrogen bonding (Applications to be discussed with relevant topics).

Acidity and basicity of organic compounds, comparison of pK_a values of different classes of organic compounds, comparison of proton abstraction ability of commonly used bases in organic reaction.

Unit 2: Stereochemistry (10 Lectures)

Fischer, Newmann and Sawhorse Projection formula and their interconversions; Geometrical isomerism: cis–trans , syn-anti and E/Z notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers (with or without any chiral centre), Molecules with two or more chiral-centres: Distereoisomers, meso structures, Threo-erythro notation. Racemic mixture and their resolution. Relative and absolute configuration: D/L and R/S designations (including spiro compounds, allenes and biphenyls).

Elementary idea about chemo-, regio-, stereo- selective and stereospecific reactions.

Unit 3: Reaction Intermediates and Types of Organic Reactions (6 Lectures)

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges.

Electrophiles and Nucleophiles. Comparison of strength of nucleophiles in different medium.

Chemistry of reactive intermediates (carbocation, carbanions, free radicals, carbenes, nitrenes and benzynes)

Introduction to types of organic reactions: Addition, Elimination and Substitution reactions.

Unit 4: Chemistry of Aliphatic Hydrocarbons (15 Lectures)

A. Carbon-Carbon Sigma Bonds

General methods of preparation: Wurtz Reaction, Wurtz-Fittig Reaction, Kolbe's reaction, Corey-House reaction. Physical and chemical properties of alkanes: Free radical substitutions: Halogenation (with mechanism) -relative reactivity and selectivity.

B. Carbon-Carbon Pi Bonds

General methods of preparation of alkenes and alkynes: Mechanism of E1, E2, E1cb reactions , Saytzeff and Hofmann eliminations. Physical and Chemical properties: Electrophilic addition reactions with mechanisms, addition of hydrogen halides (Markownikoff/ Anti Markownikoff addition), addition of water, addition of halogen with stereochemistry, mechanism of oxymercuration-demercuration, hydroboration- oxidation, epoxidation, ozonolysis, reduction (catalytic and chemical), syn- and anti-hydroxylation (oxidation) , Simmons-Smith reaction , 1,2-and 1,4-addition reactions in conjugated dienes. Allylic and benzylic bromination and mechanism, e.g. propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

C. Cycloalkanes and Conformational Analysis

Conformational analysis of alkanes: Relative stability and Energy diagrams. Types of cycloalkanes and their relative stability, Baeyer strain theory : Chair, Boat and Twist boat forms of cyclohexane with energy diagrams ; Relative stability of mono and di substituted cycloalkanes.

Unit 5: Aromatic Hydrocarbons (8 Lectures)

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions, heterocyclic compounds, annulenes, Tropone, fulvalenes, azulene with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Practical: 60 Hours

Unit 6: Organic Chemistry Lab (2 Credit)

1. Purification of organic compounds by crystallization using the following solvents:

   a. Water b. Alcohol c. Alcohol-Water

2. Determination of the melting points of unknown organic compounds (electrically heated melting point apparatus)

3. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds

4. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)

5. Qualitative organic analysis (test for aliphatic/aromatic, test for saturation/unsaturation, Lassaign test, test for functional groups, determination of melting point of the unknown compound, preparation of derivative and determination of melting point of the prepared derivative, identification of the organic sample).
[Five samples should be analysed by each student]

List of Suggested Books:

1. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press.
2. R. N. Morrison and R. N. Boyd. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. I. L. Finar, Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. E. L. Eliel, Basic Organic Stereochemistry (Wiley)
5. P. S. Kalsi. Stereochemistry, Conformation and Mechanism New Age International.
6. A.K Nad, Ghosal and Mahapatra. An Advanced Course in Practical Chemistry (New Central Book Agency)

Paper: CHM202C (Core)
Physical Chemistry II

Credits: 5=4+0+1 (60 Lectures)

Theory: 60 Lectures

Unit 1: Chemical Thermodynamics – II (24 Lectures)

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

Helmholtz and Gibbs free energy functions, their significance about the direction of spontaneous changes, their dependence respectively on (V,T) and on (P,T). Maxwell's relations and the derivation of thermodynamic equation of state. Gibbs-Helmholtz equation – involving the Gibbs free energy G itself and the Gibbs free energy of a reaction, $\Delta_r G$.

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. Change in chemical potentials and Gibbs function during mixing of non-reacting ideal gases.

The Nernst heat theorem and third law of thermodynamics, concept of residual entropy, calculation of absolute entropy of substances.

Criteria of thermodynamic equilibrium, criterion of chemical equilibrium in terms of G, concept of degree of advancement of a reaction. Standard enthalpy, entropy, and Gibbs function of reactions – these for formation and combustion reactions. Thermodynamic derivation of relation between Gibbs free energy of reaction $\Delta_r G$ and reaction quotient Q_c; and of the relation between $\Delta_r G°$ and the equilibrium constant K_c. The equilibrium constants K_c, K_p and K_x for gas-phase reactions and their inter-relations. Dependence of equilibrium constant on temperature and pressure – quantitative aspect of the Le Chatelier principle.

Unit 2: Electrochemical Cells (21 Lectures)

Electrochemical cells: measurement of cell EMF and electrode (half-cell) potentials, concept of SHE as the primary reference electrode, electrode-potential sign convention, different classes of electrodes, the calomel electrodes (SCE, NCE and DNCE) and their use as secondary reference electrodes. Rules of oxidation/reduction of ions based on half-cell potentials; conventions for

designating anode and cathode for electrolytic and Galvanic cells. Dependence of electrode potential and cell EMF on the concentrations – the Nernst equation. Distinction between chemical cells and concentration cells, concentration cells with and without transference; the liquid junction potential; expressions for EMF and the liquid junction potential for concentration cells.

Application of EMF measurements for determining (i) the free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants (iii) activity coefficients and (iv) pH values (using quinhydrone and glass electrodes). Interpretation of polarography. Qualitative discussion of potentiometric acid-base titrations using glass electrode.

Primary cells: construction and working of zinc-graphite dry cells (acidic and alkaline). Secondary cells: construction and working of lead-acid battery. Fuel cells – phosphoric acid and aqueous alkali fuel cells as illustrations, their applications and reason behind their high efficiency.

Electrochemical basis of corrosion in metals, measures for its prevention.

Unit 3: Solutions and Colligative Properties (15 Lectures)

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, calculation of molar masses of normal, dissociated and associated solutes in solution.

Thermodynamic derivation using chemical potential of relations for the four aforesaid colligative properties. Real solutions: activity and activity coefficient, derivation of the relation analogous to the Raoult's law for solvent.

Practical: 30 Hours

Unit 4: Physical Chemistry Lab (1 Credit)

(1) Determination of the strength of a supplied CH_3COOH solution by its pH-metric titration against a NaOH solution standardised with standard oxalic acid solution.

(2) Determination of the strength of a supplied HCl solution by its conductometric titration against a NaOH solution standardised with standard oxalic acid solution.

(3) Determination of partial molar volume of ethanol for ethanol-water solutions by density measurements using a pyknometer.

List of Suggested Books:

1. Atkins's Physical Chemistry by P. Atkins and J.D. Paula (Oxford University Press)
2. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)
3. A Textbook of Physical Chemistry (Volume 1) by K.L. Kapoor (MacMillan)
4. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra (New Central Book Agency)

Paper Code – CHM203G (General Elective)
Chemistry – II

Credits: 4=3+0+1 (45 Lectures)

Theory: 45 Lectures

Unit 1: Atomic and Molecular Structure (15 Lectures)

Schrodinger's 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 wavefunction and angular wavefunction.

Many electron atoms: Effective nuclear charge, screening effect. Electron spin and spin quantum numbers. Electronic configuration of atoms, Aufbau principle, Pauli's principle, Hund's rule.

Valence bond theory of molecules: Lewis electron pair bonds (in H_2, HF, O_2, N_2, H_2O). 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). Hybridisation of atomic orbitals. Resonance (as in C_6H_6, O_3, CO_3^{2-}, NO_3^-), resonance energy, delocalisation of electrons in benzene.

Polar molecules: concept of electronegativity. Dipole moment and bond moment (as in CO_2, H_2O, NH_3, NF_3). Percentage ionic character of bonds (as in HCl).

Unit 2: States of Matter (20 Lectures)

Gases: Distribution of molecular speeds – 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. Deviation from ideal behaviour, van der Waals equation of state and its explanation, critical phenomena and critical constants.

Liquids: Properties of liquids, definition of vapour pressure and its significance in deciding volatility and boiling point, concept of surface tension and viscosity. Variation of these three properties with temperature.

Solids: Crystal lattices, unit cells, the seven crystal systems and fourteen Bravais lattices. Density expressions for simple cubic, fcc and bcc lattices. Closed packed structures, octahedral and tetrahedral voids in fcc lattices. Structure of some 1:1 binary ionic solids: the CsCl, NaCl (rock salt) and cubic ZnS (zinc blende) structures. Radius ratio and coordination number in ionic solids, their role in deciding the ionic solid structure.

Unit 3: Chemical Kinetics (10 Lectures)

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

Practical: 30 Hours

Unit 4: Elective Chemistry Lab (1 Credit)

General Chemistry Experiments:

(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.

List of Suggested Books:

1. General Chemistry by D. D. Ebbing and S. D. Gammon
2. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)
3. College Practical Chemistry by V. K. Ahlualia, S. Dhingra and S. Gulati (Universities Press)