

CORE COURSE (HONOURS) IN CHEMISTRY

SEMESTER-I

CEMACOR01T: ORGANIC CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Marks: 50

**Basics of Organic Chemistry Bonding and Physical Properties
(25 Lectures) Marks: 20**

Valence Bond Theory: concept of hybridisation, shapes of molecules, resonance (including hyperconjugation); calculation of formal charges and double bond equivalent (DBE); orbital pictures of bonding (sp^3 , sp^2 , sp : C-C, C-N & C-O systems and *s-cis* and *s-trans* geometry for suitable cases).

Electronic displacements: inductive effect, field effect, mesomeric effect, resonance energy; bond polarization and bond polarizability; electromeric effect; steric effect, steric inhibition of resonance.

MO theory: qualitative idea about molecular orbitals, bonding and antibonding interactions, idea about σ , σ^* , π , π^* , n – MOs; basic idea about Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; interpretation of chemical reactivity in terms of FMO interactions; sketch and energy levels of π MOs of i) acyclic p orbital system (C=C, conjugated diene, triene, allyl and pentadienyl systems) ii) cyclic p orbital system (neutral systems: [4], [6]-annulenes; charged systems: 3-,4-,5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram; elementary idea about α and β ; measurement of delocalization energies in terms of β for buta-1,3-diene, cyclobutadiene, hexa-1,3,5-triene and benzene.

Physical properties: influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle strain (Baeyer's strain theory); melting point/boiling point and solubility of common organic compounds in terms of covalent & non-covalent intermolecular forces; polarity of molecules and dipole moments; relative stabilities of isomeric hydrocarbons in terms of heat of hydrogenation, heat of combustion and heat of formation.

**General Treatment of Reaction Mechanism I
(10 Lectures)**

Marks: 10

Mechanistic classification: ionic, radical and pericyclic (definition and example); reaction type: addition, elimination and substitution reactions (definition and example); nature of bond cleavage and bond formation: homolytic and heterolytic bond fission, homogenic and heterogenic bond formation; curly arrow rules in representation of mechanistic steps; reagent type: electrophiles and nucleophiles (elementary idea); electrophilicity and nucleophilicity in terms of FMO approach.

Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes: generation and stability, structure using orbital picture and electrophilic/nucleophilic behavior of reactive intermediates (elementary idea).

Stereochemistry I

(25 Lectures)

Marks: 20

Bonding geometries of carbon compounds and representation of molecules: tetrahedral nature of carbon and concept of asymmetry; Fischer, sawhorse, flying-wedge and Newman projection formulae and their inter translations.

Concept of chirality and symmetry: symmetry elements and point groups (C_{av} , C_{nh} , C_{nv} , C_n , D_{ah} , D_{nh} , D_{nd} , D_n , $S_n(C_s, C_i)$); molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types).

Relative and absolute configuration: D/L and R/S descriptors; erythro/threo and meso nomenclature of compounds; syn/anti nomenclatures for aldols; E/Z descriptors for C=C, conjugated diene, triene, C=N and N=N systems; combination of R/S- and E/ Z-isomerisms.

Optical activity of chiral compounds: optical rotation, specific rotation and molar rotation; racemic compounds, racemisation (through cationic, anionic, radical intermediates and through reversible formation of stable achiral intermediates); resolution of acids, bases and alcohols via diastereomeric salt formation; optical purity and enantiomeric excess; invertomerism of chiral trialkylamines.

Reference Books

1. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
2. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
3. Sykes, P., *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
4. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
5. Carey, F. A., Giuliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012.
6. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.

7. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
 8. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
 9. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
 10. Fleming, I. *Molecular Orbitals and Organic Chemical Reactions*, Reference/Student Edition, Wiley, 2009.
 11. James, J., Peach, J. M. *Stereochemistry at a Glance*, Blackwell Publishing, 2003.
 12. Robinson, M. J. T., *Stereochemistry*, Oxford Chemistry Primer, Oxford University Press, 2005.
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CEMACOR01P: ORGANIC CHEMISTRY-I LAB
(60 Lectures/Contact Hours)

Marks: 25

1. Separation, based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO₃, etc., of components of a binary solid mixture; purification of **any one** of the separated components by crystallization and determination of its melting point. The composition of the mixture may be of the following types: Benzoic acid/*p*-Toluidine; *p*-Nitrobenzoic acid/*p*-Aminobenzoic acid; *p*-Nitrotoluene/*p*-Anisidine; etc.

2. Determination of boiling point of common organic liquid compounds e.g., ethanol, cyclohexane, chloroform, ethyl methyl ketone, cyclohexanone, acetylacetone, anisole, crotonaldehyde, mesityl oxide, etc. [Boiling point of the chosen organic compounds should preferably be less than 160 °C]

3. Identification of a Pure Organic Compound

Solid compounds: oxalic acid, tartaric acid, citric acid, succinic acid, resorcinol, urea, glucose, cane sugar, benzoic acid and salicylic acid

Liquid Compounds: formic acid, acetic acid, methyl alcohol, ethyl alcohol, acetone, aniline, dimethylaniline, benzaldehyde, chloroform and nitrobenzene

Reference Books

1. Bhattacharyya, R. C, *A Manual of Practical Chemistry*.
 2. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, CBS Publishers and Distributors.
 3. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
 4. Furniss, B.S., Hannaford, A.J., Smith, P.W.G., Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012).
 5. Dutta, S, B. Sc. *Honours Practical Chemistry*, Bharati Book Stall.
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CEMACOR02T: PHYSICAL CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Marks: 50

Kinetic Theory and Gaseous state

(20 Lectures)

Marks: 16

Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Rate of collision on wall and rate of effusion.

Maxwell's distribution of speed and energy: Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy $\geq \epsilon$, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

Chemical Thermodynamics

(25 Lectures)

Marks: 20

Zeroth and 1st law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy and statement of first law; enthalpy, H ; relation between heat capacities, calculations of q , w , U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions; Joule's experiment and its consequence

Thermochemistry: Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of $\oint dQ/T$ and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; Auxiliary state functions (G and A) and their variation with T, P and V. Criteria for spontaneity and equilibrium.

Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations

Chemical kinetics

(15 Lectures)

Marks: 14

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and n-th order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, parallel reactions and consecutive reactions (with explanation of kinetic and thermodynamic control of products; all steps first order) ; Rate equation for the fast reaction

Role of T and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, LineweaverBurk plot, turn-over number

Autocatalysis; periodic reactions

Reference Books

1. Atkins, P. W. & Paula, J. de *Atkins' Physical Chemistry*, Oxford University Press
2. Castellan, G. W. *Physical Chemistry*, Narosa
3. McQuarrie, D. A. & Simons, J. D. *Physical Chemistry: A Molecular Approach*, Viva Press
4. Engel, T. & Reid, P. *Physical Chemistry*, Pearson
5. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill
6. Maron, S. & Prutton *Physical Chemistry*
7. Ball, D. W. *Physical Chemistry*, Thomson Press
8. Mortimer, R. G. *Physical Chemistry*, Elsevier
9. Laidler, K. J. *Chemical Kinetics*, Pearson
10. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry*
11. Rakshit, P.C., *Physical Chemistry* Sarat Book House

12. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill
 13. Rastogi, R. P. & Misra, R.R. *An Introduction to Chemical Thermodynamics*, Vikas
 14. Klotz, I. M. & Rosenberg, R. M. *Chemical Thermodynamics*, Wiley
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CEMACOR02T: PHYSICAL CHEMISTRY-I LAB

(60 Lectures/Contact Hours)

Marks: 25

Experiment 1: Determination of pH of unknown solution (buffer), by color matching method

Experiment 2: Determination of heat of neutralization of a strong acid by a strong base

Experiment 3: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate

Experiment 4: Study of kinetics of decomposition of H_2O_2

Experiment 5: Determination of heat of solution of oxalic acid from solubility measurement

Reference Books

1. Viswanathan, B., Raghavan, P.S. *Practical Physical Chemistry* Viva Books (2009)
2. Mendham, J., A. I. Vogel's *Quantitative Chemical Analysis* 6th Ed., Pearson
3. Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. *Practical Physical Chemistry* Science Book Agency
5. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited *Findlay's Practical Physical Chemistry* Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., *Advanced Experimental Chemistry* S. Chand & Co. Ltd.