

### Course: Discipline Specific Core 1

Semester	<b>1</b>	
Paper Number	<b>HCHCR1012T (60 MARKS) &amp; HCHCR1012P (40 MARKS)</b>	
Paper Title	<b>CORE COURSE 1: ORGANIC CHEMISTRY</b>	
No. of Credits	<b>Theory-04, Practicals-02</b>	
Theory/Composite	Composite	
No. of periods assigned	Th: 4 Pr: 3	
Name of Faculty member(s)	Dr. Ankur Ray Prof. Dipankar Das	
Course description/objective	<p><b>Theory:</b>  <i>To have basic knowledge about the introductory concepts of Organic Chemistry, stereochemistry and reaction mechanisms</i></p> <p><b>Practical:</b>  <i>To identify the special elements and functional groups in an unknown organic sample.</i></p>	
Syllabus	Annexure Core Course: 1	
Texts		
Reading/Reference Lists	<p><b>Theory:</b></p> <ol style="list-style-type: none"> <li>1. Clayden, J., Greeves, N. &amp; Warren, S. <i>Organic Chemistry</i>, Second edition, Oxford University Press, 2012.</li> <li>2. Keeler, J., Wothers, P. <i>Chemical Structure and Reactivity – An Integrated approach</i>, Oxford University Press.</li> <li>3. Sykes, P. <i>A guidebook to Mechanism in Organic Chemistry</i>, Pearson Education, 2003.</li> <li>4. Smith, J. G. <i>Organic Chemistry</i>, Tata McGraw-Hill Publishing Company Limited.</li> <li>5. Carey, F. A., Giuliano, R. M. <i>Organic Chemistry</i>, Eighth edition, McGraw Hill Education, 2012.</li> <li>6. Eliel, E. L. &amp; Wilen, S. H. <i>Stereochemistry of Organic Compounds</i>, Wiley: London, 1994.</li> <li>7. Nasipuri, D. <i>Stereochemistry of Organic Compounds</i>, Wiley Eastern Limited.</li> <li>8. Morrison, R. N. &amp; Boyd, R. N. <i>Organic Chemistry</i>, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).</li> <li>9. Finar, I. L. <i>Organic Chemistry (Volume 1)</i>, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)</li> <li>10. Fleming, I. <i>Molecular Orbitals and Organic Chemical Reactions</i>, Reference/Student Edition, Wiley, 2009.</li> <li>11. James, J., Peach, J. M. <i>Stereochemistry at a Glance</i>, Blackwell Publishing, 2003.</li> <li>12. Robinson, M. J. T., <i>Stereochemistry</i>, Oxford Chemistry Primer, Oxford University Press, 2005.</li> </ol> <p><b>Practical:</b> Nad, Mahapatra, Ghosal-Practical Chemistry</p>	
Evaluation	<b>Theory: 60 marks</b>	<b>Practical: 40 marks</b> <i>(Continuous Assessment)</i>
	CIA: 10 End-Sem: 50	Internal Assessment Exams: 30 Viva (End Sem): 8 Attendance: 2
Paper Structure for the End Sem <b>Theory Exam</b> (50 marks)	6 (SIX) Questions (each of 10 marks) will be set and the students will have to answer any 5 (FIVE). Each of the Questions (10 marks) will consist of 2 or 3 parts (of 2/ 3/ 4/ 5 )	

**Annexure Core Course (CC): 1**  
**(Credits: Theory-04, Practicals-02)**

**Theory: 60 Lectures**

**Basics of Organic Chemistry**

**Bonding and Physical Properties**

**(25 Lectures)**

*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 effects and their influence on acidity-basicity: 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  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ ,  $n$  – 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  $\pi$  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.

*Physical properties:* influence of hybridization on bond properties: bond dissociation energy (BDE) and bond energy; bond distances, bond angles; concept of bond angle; 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)**

*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)

*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, 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: ( $n$ =odd and  $n$ = even) 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:* Concept of plane polarised light and polarimeter, 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.

## CC: 1 (Practical) 42 Lectures

1. **Separation**, based upon solubility, by using common laboratory reagents like water (cold, hot), dil. HCl, dil. NaOH, dil. NaHCO<sub>3</sub>, 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.