Course: Discipline Specific Core 4

Semester	**2**
Paper Number	**HCHCR2042T (60 MARKS) & HCHCR2042P (40 MARKS)**
Paper Title	**CORE COURSE IV: ORGANIC CHEMISTRY**
No. of Credits	**Theory-04, Practicals-02**
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	***Theory:*** ***To have knowledge about the advanced concepts of Streochemistry, reaction mechanisms including substitution and elimination reactions*** ***Practical:*** ***To identify the special elements and functional groups in an unknown organic sample.***
Syllabus	Annexure Core Course: 4
Texts	
Reading/Reference Lists	**Theory:** Clayden, J., Greeves, N., Warren, S. *Organic Chemistry,* Second edition, Oxford University Press 2012. 2. Sykes, P. *A guidebook to Mechanism in Organic Chemistry,* Pearson Education, 2003. 3. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited. 4. Carey, F. A. & Guiliano, R. M. *Organic Chemistry*, Eighth edition, McGraw Hill Education, 2012. 5. Loudon, G. M. *Organic Chemistry*, Fourth edition, Oxford University Press, 2008. 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)* Pearson Education. 10. Graham Solomons, T.W., Fryhle, C. B. *Organic Chemistry,* John Wiley & Sons, Inc. 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. 13. Maskill, H., *Mechanisms of Organic Reactions*, Oxford Chemistry Primer, Oxford University Press. ***Practical*** 1. Vogel, A. I. *Elementary Practical Organic Chemistry,* Part 1: *Small scale Preparations,* CBS Publishers and Distributors. 2. *University Hand Book of Undergraduate Chemistry Experiments*, edited by Mukherjee, G. N. University of Calcutta, 2003. 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. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis,* University Press (2000). 6. *Practical Workbook Chemistry (Honours), UGBS, Chemistry*, University of Calcutta, 2015.	
Evaluation	**Theory: 60 marks**	**Practical: 40 marks** *(Continuous Assessment)*
	CIA: 10 End-Sem: 50	Internal Assessment Exams: 30 Viva (End Sem): 8 Attendance: 2
Paper Structure for the End Sem **Theory Exam** (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): 4

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Stereochemistry II **(20 Lectures)**

Chirality arising out of stereoaxis: stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidenecycloalkanes and biphenyls; related configurational descriptors (R_a/S_a and *P/M*); atropisomerism; racemisation of chiral biphenyls; *buttressing* effect. Chiral rigidity: twistanes, point groups.

Concept of prostereoisomerism: prostereogenic centre; concept of (*pro*)^n-*chirality*: topicity of ligands and faces (elementary idea); *pro-R/pro-S, pro-E/pro-Z* and *Re/Si* descriptors; *pro-r* and *pro-s* descriptors of ligands on propseudoasymmetric centre.

Conformation: conformational nomenclature: eclipsed, staggered, *gauche*, *syn* and *anti*; dihedral angle, torsion angle; Klyne-Prelog terminology; *P/M* descriptors; energy barrier of rotation, concept of torsional and steric strains; relative stability of conformers on the basis of steric effect, dipole-dipole interaction and H-bonding; *butane gauche* interaction; conformational analysis of ethane, propane, *n*-butane, 2-methylbutane and 2,3-dimethylbutane; haloalkane, 1,2-dihaloalkanes and 1,2-diols (up to four carbons); 1,2-halohydrin; conformation of conjugated systems (*s-cis* and *s-trans*).

General Treatment of Reaction Mechanism II **(18 Lectures)**

Reaction thermodynamics: free energy and equilibrium, enthalpy and entropy factor, calculation of enthalpy change via BDE, intermolecular & intramolecular reactions.

Tautomerism: prototropy (keto-enol, nitro - *aci*-nitro, nitroso-oximino, diazo-amino and enamine-imine systems); valence tautomerism and ring-chain tautomerism; composition of the equilibrium in different systems (simple carbonyl; 1,2- and 1,3-dicarbonyl systems, phenols and related systems), factors affecting keto-enol tautomerism; application of thermodynamic principles in tautomeric equilibria.

Reaction kinetics: rate constant and free energy of activation; concept of order and molecularity; free energy profiles for one-step, two-step and three-step reactions; catalyzed reactions: electrophilic and nucleophilic catalysis; kinetic control and thermodynamic control of reactions; isotope effect: primary and secondary kinetic isotopic effect (k_H /k_D); principle of microscopic reversibility; Hammond's postulate.

Substitution and Elimination Reactions (22 Lectures)

Free-radical substitution reaction: halogentaion of alkanes, mechanism (with evidence) and stereochemical features; reactivity-selectivity principle in the light of Hammond's postulate.

Nucleophilic substitution reactions: substitution at sp^3 centre: mechanisms (with evidence), relative rates & stereochemical features: S_N1, S_N2, S_N2', S_N1' (allylic rearrangement) and S_Ni; effects of solvent, substrate structure, leaving group and nucleophiles (including ambident nucleophiles, cyanide & nitrite); substitutions involving NGP; role of crown ethers and phase transfer catalysts; [systems: alkyl halides, allyl halides, benzyl halides, alcohols, ethers, epoxides].

Elimination reactions: E1, E2, E1cB and Ei (pyrolytic *syn* eliminations); formation of alkenes and alkynes; mechanisms (with evidence), reactivity, regioselectivity (Saytzeff/Hofmann) and stereoselectivity; comparison between substitution and elimination; importance of Bredt's rule relating to the formation of C=C.

CHEMISTRY LAB-C IV LAB **60 Lectures**

Organic Preparations

A. The following reactions are to be performed, noting the yield of the crude product:

1. Nitration of aromatic compounds

2. Condensation reactions

3. Hydrolysis of amides/imides/esters

4. Preparation of binaphthol from β-naphthol

5. Benzoylation of phenols/aromatic amines

6. Side chain oxidation of aromatic compounds

7. Diazo coupling reactions of aromatic amines

8. Bromination of anilides using green approach (Bromate-Bromide method)

9. Redox reaction including solid-phase method

10. Green 'multi-component-coupling' reaction

11. Selective reduction of *m*-dinitrobenzene to *m*-nitroaniline

Students must also calculate percentage yield, based upon isolated yield (crude) and theoretical yield.

B. Purification of the crude product is to be made by crystallisation from water/alcohol, crystallization after charcoal treatment, or sublimation, whichever is applicable.

C. Melting point of the purified product is to be noted.