

DISCIPLINE-SPECIFIC ELECTIVE COURSE - 16 (DSE-16)

Advanced Stereochemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/Practice		
Advanced Stereochemistry (DSE-16)	04	02	--	02	--	--

Learning Objectives:

To provide a comprehensive understanding of molecular symmetry, isomerism, and chirality, including their applications in organic reactions.

Learning Outcomes:

1. Students will be expected to gain knowledge of the basic concept of chirality in molecules due to their spatial arrangement of atoms that leads to chiroptical properties.
2. The three-dimensional arrangement of atoms in a molecule can lead to distinct physical and chemical properties, particularly for stereoisomers. Understanding stereochemistry is crucial for designing effective drugs, predicting reaction outcomes, and developing new materials.
3. Stereochemistry significantly impacts drug action, biological processes, and chemical reactions, influencing factors like drug efficacy, selectivity, and even the rate of chemical reactions.

SYLLABUS OF DSE 16

Unit 1: (Hours:15)

Stereoisomerism: Chiral (stereogenic) centre, principle of axial and planar chirality; Stereochemistry and configurations of biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes, allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes and helicity.

Unit 2: (Hours: 5)

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic and prochiral centres.

Unit 3: (Hours: 5)
Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (di-, and tri-substituted), cyclohexenes, cyclohexanones, decalin.

Unit 4: (Hours:5)
Asymmetric induction: Cram's, Prelog's, and Felkin-Ahn model. Applications of ORD and CD to Stereochemical Problems

Practical Component

(Any 10 practicals may be done depending upon the availability of resources.)

1. E/Z and Cis-Trans Isomerism of 2,3-dimethyl-2-butene by ball and stick models
2. Identification of ChiralCentres and Diastereomers by ball and stick models
3. Bromination of cis and trans stilbene
4. Addition of Bromine to trans-Cinnamic Acid
5. Photoinduced isomerization of *cis*-Stilbene to *trans*-Stilbene and *vice versa*
6. Photocatalytic/ thermal isomerization of maleic acid to fumaric acid.³
7. Preparation of stilbene dibromide by bromination of *trans*-stilbene.
8. Determination of optical rotation of sucrose, glucose, and fructose using polarimetry and determining their concentration.
9. Two-step synthesis of acetonide from benzil and analysis of its stereochemistry using NMR and IR spectroscopy
10. Determination of specific rotation of (R)-limonene and (S)-limonene using Polarimeter.
11. Preparation of hydroxybenzoin by pinacol coupling reaction: Investigating the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: Affording *meso*- and *dl*-Hydrobenzoin.⁴
12. Proline-catalyzed aldol reaction of cyclohexanone with nitro-substituted benzaldehydes.⁵

Recommended Reference and Textbooks: (For Theory)

1. Eliel, E. L. (2000), Stereochemistry of Carbon Compounds, Tata McGraw-Hill.
2. Nasipuri, D.(2018), Stereochemistry of Organic Compounds: Principles and Applications, 4th Edition, New Age International.

For Practical

- 1 Microscale Organic Laboratory (Multistep and Multiscale Syntheses). By Dana W. Mayo, Ronald M. Pike, David C. Forbes. **2011**.
- 2 Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments, Kenneth M. Doxsee, James E. Hutchison. Thomson-Brooks/Cole, **2004**.
- 3 The photochemical isomerization of maleic to fumaric acid: an undergraduate organic chemistry experiment. Albert J. Castro, Suzanne R. Ellenberger, and James P. Sluka. *J. Chem. Edu.* **1983**, *60* (6), 521 (DOI: 10.1021/ed060p52).

4 Using ^1H NMR Spectroscopy to Investigate the Diastereoselectivity of Benzaldehyde Pinacol Coupling Mediated by Al-KOH in Aqueous Media: An Undergraduate Lab Experiment Involving a Green Carbon–Carbon Bond-Forming Reaction Affording *meso*- and *dl*-Hydrobenzoins. Shahrokh Saba; Isabella Fante; James A. Cordero Jr. *J. Chem. Educ.* 2025, 102, 2, 847–851) doi.org/10.1021/acs.jchemed.4c01379

5 Proline-catalyzed asymmetric reactions. List, Benjamin. *Tetrahedron*. 2002, 58 (28): 5573–5590. doi:10.1016/S0040-4020(02)00516-1
