

DISCIPLINE SPECIFIC ELECTIVE COURSE – 5 (DSE-5): Reactions, Reagents and Chemical Process

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		
Reactions, Reagents and Chemical Process (DSE-5)	04	03	--	01	Class 12 th with Physics, Chemistry	Basic knowledge of organic reactions

Learning objectives

The objectives of this course are as follows:

- To study the important organic name and rearrangement reactions that are crucial for the synthesis of valuable organic compounds.
- To give the knowledge belonging to the role of reagents in organic reactions for the synthesis of chemo-, diastereo- and enantio-selective products.
- To impart the knowledge of process chemistry that is a key part of the large-scale synthesis of chemical products essential for day-to-day life

Learning outcomes

By studying this course, students will be able to:

- Explain the reaction mechanism of various name and rearrangement reactions
- Discuss the role of the reagents in organic synthesis and apply these reagents for the bulk chemical synthesis
- Debate and use oxidizing and reducing reagents for selective synthesis organic products
- Apply the learnt techniques to chemical processes
- Acquire skills for human resource building especially in the chemical industry.

SYLLABUS OF DSE-5

UNIT – 1: Name Reactions

(15 Hours)

Application, scope and mechanism of following reactions: Prevost Reaction, Chugaev Reaction, Maukaiyama Aldol Reaction, Mozingo Reaction, Ramberg Backlund Reaction, Shapiro Reaction, Barbier Reaction, Clark- Eschweiler Reaction, Darzen's Reaction, Julia-Olifination Reaction, Tiffeneaus Damjanov Reaction, Darkin West Reaction, Bischler-Napieralaski Reaction, Birch reduction of aromatic compounds, Appel Reaction, Mitsunobu

Reaction, Corey Kim Oxidation, Azide-alkyne 1,3-dipolar cycloaddition reaction, Olefin metathesis: Grubbs reaction, Heck Reaction, Suzuki coupling and Wittig reaction.

UNIT – 2: Reducing Reagents

(9 Hours)

Reactions, mechanism and applications of following reducing agents: Sodium borohydride, Lithium aluminium hydride, NaBH_3CN , DIBALH, lithium-tri-*tert*-butoxyaluminum hydride, Red-Al $\text{Na}[\text{AlH}_2(\text{OCH}_2\text{OCH}_2\text{OCH}_3)_2]$, Zinc borohydride, L and K selectrides, LiBHEt_3 and KBHEt_3 , Luche Reagent $\text{NaBH}_4\text{-CeCl}_3$, $\text{K}[\text{BH}(\text{OAc})_3]$, *bis*-Boric Acid (BBA), Catecholborane, DEMS (Diethoxymethylsilane), 3-Mercapto propionic acid, Polymethylhydrosiloxane (PMHS), Schwartz's Reagent (Zirconocene chloride hydride).

UNIT – 3: Oxidizing Reagents

(9 Hours)

Reactions, mechanism and applications of following oxidizing agents: Jones Reagent (CrO_3 , H_2SO_4 , H_2O), Swern Reagent (DMSO, oxalyl chloride), Dess Martin, TEMPO, TPAP (Tetrapropyl ammonium perruthenate), Fetizon's Reagent, Fenton's Reagent [H_2O_2 + $\text{Fe}(\text{II})$ ion], Sodium perborate NaH_2BO_4 , Sodium Bismuthate NaBiO_3 , ABNO (9-Azabicyclo[3.3.1]nonane N-oxyl), DEAP (Diethyl allyl phosphate, $\text{CH}_2=\text{CH}-\text{CH}_2-\text{OPO}(\text{OEt})_2$), AZADO (2-Azaadamantane N-oxyl), Wacker oxidation.

UNIT – 4: Process Chemistry

(12 Hours)

1. Process chemistry a) Introduction, stages of scale up process: Bench, pilot, and large-scale process with at least two examples of scale up process of API. b) In-process control and validation of large-scale process.
2. Unit Processes: The following unit processes should be studied with mechanism and one example of each process Nitration: Nitrating agents, process equipment for technical nitration. Halogenation: Types of halogenations, catalytic halogenations. Reduction: Catalytic hydrogenation, hydrogen transfer reactions, metal hydrides. Oxidation: Types of oxidative reactions, and non-metallic oxidizing agents such as H_2O_2 , sodium hypochlorite, oxygen gas, ozonolysis.

Practical component

Credits:

01 (Laboratory periods:15 classes of 2 hours each)

1. Oxidation of alcohols to acid using Jones reagent.
2. Reduction of acetophenone and its derivatives to 1-phenyl ethanol derivatives by NaBH_4 .
3. Reduction of 4-*tert*-butyl-cyclohexanone to *cis* and *trans* 4-*tert*-butyl-cyclohexanol.
4. Synthesis of 2,5-dimethyl-2,5-hexanediol from *tert*-butanol using Fenton's reagents.
5. Wittig reaction of benzyltriphenylphosphonium chloride and 4-bromobenzaldehyde using potassium phosphate (tribasic).
6. Substitution ($\text{S}_{\text{N}}2$) reaction of 1-iodobutane and 2-naphthol.
7. Aldol condensation reaction: solventless synthesis of chalcones.
8. Borohydride reduction of a ketone: hydrobenzoin from benzil.
9. Visit to chemical industry of the demonstration of pilot scale.

Essential/recommended readings

Theory:

2. Clayden, J. Greeves, N., Warren, S. **Organic Chemistry**, South Asian Edition, Oxford University Press, USA
3. Gadamasetti K., **Process Chemistry in the Pharmaceutical Industry: Challenges in an Ever- Changing Climate-An Overview**, Vol-2, CRC Press, London.
4. Murphy R.M., **Introduction to Chemical Processes: Principles, Analysis, Synthesis**, McGraw-Hill Education, New York.
5. Harrington P. J., **Pharmaceutical Process Chemistry for Synthesis: Rethinking the Routes to Scale up**, John Wiley and Sons, Inc, New Jersey.
6. Parashar, R.K.; Ahluwalia, V.K. (2018), **Organic Reaction Mechanism**, 4th Edition, Narosa Publishing House.

Practical:

1. Mann F.G, Saunders, B.C., **Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.
2. Vogel A.I., **Elementary Practical Organic Chemistry**, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education Ltd.), Singapore.

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.