## DISCIPLINE SPECIFIC CORE COURSE - 20 (DSC-20): Catalysis, Photocatalysis, Application of Reagents in Organic Synthesis and Statistical Thermodynamics

### 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 | | |
| Catalysis, Photocatalysis, Application of Reagents in Organic Synthesis and Statistical Thermodynamics **(DSC-20)** | **04** | **03** | **--** | **01** | **Class 12th with Physics, Chemistry, Maths** | **--** |

### Course Objectives

**The objectives of this course are as follows:**

- To imparts basic knowledge of Organometallic compounds and catalysis,
- To enrich students with the knowledge of various types of bonding and structure of organometallic compounds and biocatalysts.
- To impart the theoretical and practical knowledge of catalysts with the view of their industrial applications.
- To facilitate chemical transformations by providing the necessary conditions and catalysis.
- To provide a brief foundational understanding of the core principles of statistical thermodynamics.
- To study the connection between macroscopic thermodynamics and microscopic quantum mechanics utilizing various statistical ensembles.
- To study Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics with a brief, qualitative understanding and focus on their applications.
- To enable students to apply statistical concepts in key areas such as the standard model, chemical kinetics, and chemical equilibrium.

### Learning outcomes

**By studying this course, the students will be able to:**

- Develop understanding on of the role of catalyst in industrial applications.

- Gain sound knowledge of various types of catalyst.
- Develop skilled in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
- Develop skilled concepts of industrial catalysis which will help them to explore new innovative areas of research
- Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.
- Understand the conversion of specific functional groups without affecting others and maximize yields and selectivity for the desired products
- Understand the fundamental principles of statistical mechanics, including how they link microscopic behaviour to macroscopic properties of systems.
- Apply the Boltzmann distribution, Bose-Einstein statistics, and Fermi-Dirac statistics in various physical and chemical systems.
- Analyse and solve problems related to the thermodynamic properties of systems using partition functions.
- Explore the application of statistical mechanics to key areas such as chemical kinetics, chemical equilibrium, and random walk models in macromolecular systems.

**UNIT- 1: Catalysis and Photocatalysis (15 Hours)**

General principles of catalysis, properties of catalysts, Mode of action of catalyst, Types of catalyst (homogeneous and heterogeneous catalysis), Deactivation and regeneration of catalysts, catalytic poison, Promoter, Turnover frequency, Turnover number, Specificity and selectivity.

Catalysis in environmental remediation, eco-friendly energy solutions and production of valuable chemicals.
Study of the following industrial processes, catalytic cycle and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst).
2. Synthetic gasoline (Fischer Tropsch reaction).
3. Polymerisation of ethene using Ziegler-Natta catalyst.
4. Wacker-Smith synthesis of aldehyde.

*Photocatalysis:* Basic principle, Mechanism, Types of Photocatalysts, band gap, tuning of band gap, doping, UV- visible light lamp source, UV-visible light filters, Water Splitting, Photoreduction and oxidation of water, Brief discussion of example of Photocatalysis: Photosynthesis, Pollutant degradation, Hydrogen production, $CO_2$ conversion.

**UNIT- 2: Synthesis and applications of Reagents in Organic Synthesis (15 Hours)**

Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents.

Triacetoxyborohydride, Lead Acetate, Phenyliodine (III) diacetate (PIDA), DCC, Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification & Swern Oxidation); Oxidation of organic compounds using thallium nitrate, selenium dioxide, phase transfer catalyst, crown ethers, $KMnO_4$, PCC, $OsO_4$, $CrO_3$, $K_2Cr_2O_7$.
Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN.

**UNIT- 3: Elements of Statistical Mechanics (10 Hours)**

Microstates, Configurations, tossing of coins, rolling of dices and spin of electrons in absence of magnetic field, most probable thermodynamic probability, Stirling's Approximation, Concepts of ensembles, Microcanonical, Canonical ensembles, Qualitative Discussion of translational, vibrational, and rotational Partition functions, Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac Statistics (Qualitative discussions)

**UNIT- 4: Conventional Transition State Theory and Brownian Motion (5 Hours)**

Conventional transition state theory in terms of molecular partition functions, gas phase equilibrium constant in terms of partition function, 1-D random walk model, Brownian Dynamics (Qualitative discussion only).

**Practicals: Credits: 01**

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

**PART A : INORGANIC CHEMISTRY**

1. Synthesis of "Zeolite A" catalyst.
2. Zeolite Hydrogen-Y or dil.HC1/dil.$H_2SO_4$ as a Catalyst for the Preparation of an Ester.
3. Catalytic Synthesis of biaryl.
4. Catalytic Transfer Hydrogenation of Castor Oil
5. Reduction of Nitrobenzene
6. Synthesis of $Cu_2O$, $TiO_2$, $Fe_3O_4$, ZnO, and NiO Nanoparticles and characterization by UV/Vis spectroscopy.
7. Photocatalytic degradation of Methylene Blue dye using $Cu_2O$, $TiO_2$, $Fe_3O_4$, ZnO, and NiO Nanoparticles and UV/Vis studies.

**PART B : ORGANIC CHEMISTRY**

8. Identification of the product based on Melting point and spectroscopic techniques (IR, $^1$HNMR, and $^{13}$C NMR spectroscopy, data to be provided).
9. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
10. Reduction of *p*-nitrobenzaldehyde using $NaBH_4$
11. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
12. Oxidation of benzyl alcohol by $KMnO_4$.

**PART C: PHYSICAL CHEMISTRY**

13. Study of kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method.*
14. Statistical Treatment of Error Analysis (Null Hypothesis, T-test, F-test, Q-test (criteria for rejection of hypothesis) Statistical analysis of laboratory data.

15. Determination of standard deviation, mean, and maximum absolute errors, root-mean-square deviation (error), and Correlation coefficient of linear straight-line plot.

**Essential/recommended readings**

**Theory:**


1. Huheey, J. E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
2. Cotton, F.A.; Wilkinson, G. (1999), Advanced Inorganic Chemistry, Wiley-VCR.
3. Jens Hagen (2015) Industrial Catalysis: A Practical Approach Wiley-VCR Verlag GmbH&Co
4. Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (1996).
5. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
6. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (2000)
7. McQuarrie, D. A. *Statistical Mechanics,* Viva Books Pvt. Ltd.: New Delhi (2003).
8. Reif, Frederick., Fundamentals of Statistical and Thermal Physics, McGraw-Hill, (1965).
9. Huang, Kerson, Statistical Mechanics, 2nd ed., Wiley (1987).
10. Pathria, R. K., and Paul D. Beale, Statistical Mechanics, 3rd ed., Elsevier (2011).
11. Pal, Palash B., (2008) Statistical Mechanics: Principles and Applications, Narosa Publishing House.
12. Bagchi B., (2018) Statistical Mechanics for Chemistry and Material Science, CRC Press.
13. L. D. Landau and E. M. Lifshitz, (2005) Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed.
14. Laidler, K. J. (1997) *Chemical Kinetics* 3rd Ed., Benjamin Cummings.
15. Atkins, P. W. & Paula, J. de (2006) *Atkin's Physical Chemistry* 8th Ed., Oxford University Press.
16. McQuarrie, D. A. & Simon, J. D. (2001) *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books.


**Practical:**


1. Williams, D. J.; Huck, B. E.; Wilkinson, A. P. First-Year Undergraduate Laboratory Experiments with Zeolites Chem. Educator 2002, 7, 33-36.
2. Coker, E. N.; Davis, P. J.; Experiments with Zeolites at the Secondary-School Level: Experience from The Netherlands Journal of Chemical Education 1999, 76, 10, 1417.
3. Hanson RW. Catalytic transfer hydogenation reactions for undergraduate practical programs. J Chem Educ. 2009, 74, 430.
4. Alwaseem H, Donahue CJ, Marincean S. Catalytic transfer hydrogenation of castor oil. J Chem Educ. 2014; 91, 575-8.
5. Ramesh R; Rajendran A.; Photocatalytic dye degradation activities of green synthesis of cuprous oxide nanoparticles from Sargassum wightii extract, Chemical Physic Impact, 2023, 6, 100208.

6. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
7. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
8. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
9. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi
10. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
11. McQuarrie, D. A. & Simon, J. D. (2001) *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books.

**Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.**