Semester VIII

DISCIPLINE SPECIFIC CORE COURSE - 20 (DSC-20): Organometallic Chemistry and Bio- catalysis, Application of Reagents in Organic Synthesis and Crystalline Solids & their Magnetic Properties

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		
Organometallic Chemistry and Bio-catalysis, Application of Reagents in Organic Synthesis and Crystalline Solids & their Magnetic Properties **(DSC-20)**	**04**	**03**	**--**	**01**	**Class 12th with Physics, Chemistry**	**--**

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 analyze different crystal systems and understand their properties.
- To study Curie's and Curie-Weiss law and its application to paramagnetic and ferromagnetic materials, respectively.
- To understand the principles of powder-XRD and structural analysis of solids.

Learning outcomes

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

- Understand the role of catalyst in industrial applications.
- Gain sound knowledge of various types of catalyst.
- Get skilled in the scientific method of planning, developing, conducting, reviewing and reporting experiments.

- Get 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
- Analyze the distingtion between lattice, unit cell, and the 14 Bravais lattices, and understand their symmetry and properties.
- Interpret XRD patterns of NaCl, CsCl, and KCl to deduce structural information.
- Understand the Curie-Weiss law and its application to ferromagnetic materials.
- Interpret data obtained from instrumental techniques for structural analysis of crystalline solids.

UNIT- 1: Organometallic Chemistry and Biocatalysis (15 Hours)

Definition and classification with appropriate examples based on nature of metal-carbon bond (ionic, sigma, pi and multicentre bonds), Structure and bonding of methyl lithium and Zeise's salt, Structure and bonding of ferrocene, mononuclear and polynuclear carbonyls of 3d metals, 18-electron rule as applied to carbonyls, π-acceptor behaviour of carbon monoxide (MO diagram of CO to be discussed), synergic effect and use of infrared spectroscopy data to explain the extent of back bonding. Bio-organometallic chemistry: Conjugates of ferrocene with biomolecules such as amino acid and protein, and their applications. Organometallic complexes as radiopharmaceuticals.

Key aspects of Bio-catalysis, Variables affecting bio-catalysis such as temperature, pH, solvent etc., Enzyme catalyzed reactions and their Kinetics. Detailed study of biocatalyst in the metabolism of Hydrogen, carbon, and sulfur. Nanobiocatalysis.

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: Crystalline Solids (11Hours)

Classification and characteristics of crystalline solids, seven crystal systems. Fundamentals of lattice, unit cell and fourteen Bravais lattices. Types of closed-packed structures. Elementary idea of symmetry. Crystal's direction and planes, Miller indices. X-ray diffraction, Bragg's law. PXRD diffraction pattern of NaCl, CsCl, and KCl,

UNIT -4: Magnetic Properties of Solids (4 Hours)

Magnetic moment, Curie law, Curie-Weiss law, mechanism of magnetic ordering, exchange Interaction, domain theory, hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism.

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

PART B: ORGANIC CHEMISTRY

Identification of the product based on Melting point and spectroscopic techniques (IR, ^{1}HNMR, and ^{13}C NMR spectroscopy, data to be provided).

5. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
6. Reduction of *p*-nitrobenzaldehyde using $NaBH_4$
7. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
8. Oxidation of benzyl alcohol by $KMnO_4$.

PART C: PHYSICAL CHEMISTRY

9. Analysis of diffraction pattern obtained from Powder X-ray diffractometer. Identifying crystal phase, diffraction peaks with lattice planes for a given compound.
10. Analysis of p-XRD data of a given set of Metals/ compounds* (Ag/Au/Cu/NaCl/CsCl) and confirmation of the type of the cubic system corresponding to given species.
11. Determination of approximate crystallite size using the measured PXRD pattern of a known inorganic compound i.e. TiO_2, ZnO etc by employing Scherer equation.
12. Determination of lattice strain using Williamson-Hall equation and from the measured PXRD pattern of a known inorganic compound for example, TiO_2, ZnO etc.*

*[Diffraction patterns of known sample along with Standard JCPDS file (JCPDS: Joint Committee for Powder Diffraction Studies) be provided to students for analysis]

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. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), Inorganic Chemistry, 5th Edition, Pearson.
4. Jens Hagen (2015) Industrial Catalysis: A Practical Approach Wiley VCR Verlag GmbH&Co
5. Gérard Jaouen,(2006) Bioorganometallics, Wiley-VCH Verlag GmbH & Co.
6. Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (1996).
7. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).

8. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (2000)
9. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 5th Edition, Mc Graw Hill Education.
10. Levine I.N. (2009), Physical Chemistry 6th Edition, Mc Graw Hill Education.
11. Pillai S.O., (2022) Solid State Physics 6th Edition, New Age International Publishers.
12. Chakrabarty, (2022) D. K., Solid State Chemistry, 2nd Edition, New Age International Publishers.
13. West, A.R., (2022), Solid State Chemistry and its Applications, 2nd Edition, Wiley Inc.
14. Callister W. D., (2018) Materials Science and Engineering: An Introduction, 10th Edition, Willey Inc.
15. Keer H. V., (Reprint 2005), Principles of the Solid State, New Age International Publishers.

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. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
6. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
7. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
8. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi
9. Cullity, B. D. (2001) *Elements of X-ray Diffraction*, 3rd ed.; Prentice Hall.
10. Hammond, C. (2015) *The Basics of Crystallography and Diffraction*, 4th ed.; Oxford University Press.
11. Snyder, R. L. (1996) Jenkins, R. *Introduction to X-ray Diffractometry*; Wiley: New York.
12. Hulien M.L., Lekse J.W., Rosmus K. A., Devlin K. P., Glenn J.R., Wisneski S. D., Wildfong P., Lake C. H., MacNeil J. H.Aitken J. A., An Inquiry-Based Project Focused on the X-ray Powder Diffraction Analysis of Common Household Solids, *J. Chem. Educ.* 2015, *92, 12, 2152-2156*.
13. Evans J. S. O., Evans I.R., Structure Analysis from Powder Diffraction Data: Rietveld Refinement in Excel, *J. Chem. Educ.* 2021, *98, 2, 495-505*.
14. https://www.icdd.com/ (International Centre for Diffraction Data)

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