Semester	JAN 2022
Open to semester	8,12,14,22
Course code	**CH4214/CH6424**
Course title	**Organotransition Metal Catalysis**
Credits	4 /4
Course Coordinator & participating faculty (if any)	Shabana Khan
Nature of Course	Lectures
Pre-requisites	Basic Chemistry
Objectives (goals, type of students for whom useful, outcome etc)	Catalysis is of fundamental importance in chemistry and plays a vital role in basic research, applied sciences as well as industrial processes. To understand the essence of catalysis and the relationship between catalysis effect and catalyst structure, it is important to learn the basic principles behind the metal, ligands and their bonding properties. Emphasis will be placed on structure, bonding and catalytic cycles and how they are derived from appropriate experimental data; implicit in this is a complete understanding of the fundamental reaction types prevalent in these cycles such as oxidative addition, migratory insertion, and reductive elimination; How appropriate ligand design can be used to 'tailor' catalytic properties such as reactivity and selectivity. It will serve as a foundation to apply this knowledge for a better understanding of catalysts and catalysis.
Course contents (details of topics /sections with no. of lectures for each)	1. Introduction: Catalysis - Term and basic principles, Why is catalysis required?, The development of organotransition metal catalysis, Principles of catalysis: homogenous and heterogeneous catalysis, selectivity and specificity of catalysts, general practical method for catalysis, etc. (4 hrs) 2. Structure and bonding: General properties of ligands: dative (L-type), covalent (X-type), neutral, anionic, even- or odd-electron, ?-bonded, combination of ? and ? donor, and cationic ligands. Structure and electronic properties of phosphines and N-heterocyclic carbenes, estimation of their donor strength, Tolman electronic parameter, ligands effect on catalytic efficiency. Properties of metals: oxidation state, the relationship between oxidation state and no. of d-electrons, trends in the properties of transition metals. (8 hrs)

	3. Homogeneous Catalysis and Important reactions: Elementary steps in organometallic catalysis: oxidative addition and reductive elimination, agostic interaction, ?-hydrogen elimination, ?-bond metathesis. Overview of reactions catalyzed by metal complexes in solution; Detailed discussion of the major homogeneous catalytic reactions to include hydrogenation, carbonylation, hydroformylation, hydrocyanation, hydrosilylation, hydroamination, hydroboration reactions, and a brief overview of coupling reactions including C-C, C-N coupling reactions. (10 hrs) 4. Asymmetric Catalysis: Introduction, general principle, and practical aspects of asymmetric catalysis. (3 hrs) 5. Heterogeneous Catalysis: General features, basic methods of synthesis and characterization, Ziegler-Natta catalysis: oligomerization and polymerization; Ammonia Synthesis, Fischer-Tropsch synthesis, Methane reforming and the mechanism, Zeolite catalysis, Hydrodesulfurization, Selective oxidation of propylene, Kinetics in heterogeneous catalytic reactions (8 hrs). 6. Non-classical Catalysis: Introduction of non-classical catalysis, Catalysts based on main group elements, Frustrated Lewis pair catalysts (FLPs): Basic fundamentals of FLPs and their application in small molecules activation and reduction of many functional groups, Organocatalysis: types of catalysts, examples, and mechanism, Lanthanides in catalysis, Alkali and alkaline earth metal-catalyzed reactions and mechanism. (8 hrs)
Evaluation /assessment	End-Sem Examination-50% Mid-Sem Examination-50% Others-a. End-sem examination- 35% b. Mid-sem examination-35% c. Quiz- 30% %
Suggested readings (with full list of authors, publisher, year, edn etc.)	1. Dirk Steinborn, Fundamentals of Organometallic Catalysis, Wiley-VCH . 2. John F. Hartwig, Organotransition Metal Chemistry. From Bonding to Catalysis, University Science Books, Mill Valley, California. 3. Matthias Beller, A. Renken, R. A. van Santen Catalysis. From Principles to Applications, Wiley-VCH.

	4. Gadi Rothenberg, Catalysis. Concepts and Green Applications. Wiley-VCH. 5. For Asymmetric Catalysis: Walsh, P. J., Kozlowski, M. C., Fundamentals of Asymmetric Catalysis, University Science Books, California, 2008.