

# FIRST SEMESTER 2015-2016 COURSE HANDOUT (PART-II)

Date: 03-08-2015

In addition to part I (General handout for all courses appended to the timetable) this portion gives further details regarding the course.

Course No. : CHEM F337

Course Title : Green Chemistry and Catalysis

Instructor-in-charge : BHARTI KHUNGAR

### 1. Course Description

Definition and overview of the twelve principles of Green Chemistry, alternative starting materials; alternative synthesis and reagents; E factor and the concept of atom economy; the role of catalysis, alternate energy sources (microwave & ultrasound), catalysis by solid acids and bases, bio-catalysis, catalytic reduction, catalytic oxidation, catalytic C–C bond formation, cascade catalysis, enantioselective catalysis, alternative reaction media, renewable raw materials, industrial applications of catalysis.

## 2. Scope and objective of the course:

The objectives of this course are to provide the students with a fundamental understanding of Green Chemistry with an emphasis on the design, prepare and use of chemicals and protocols that have little or no pollution potential or environmental risk. The students will also be exposed to the development of latest technologies and methodologies for environmentally benign methods which are being practiced in industry.

#### 3. Text Book:

- T1: Green Chemistry and Catalysis, Roger Arthur Sheldon, Isabel Arends, and Ulf Hanefeld, Wiley, 2007.
- T2: Green Chemistry Theory and Practice P.T Anasts and J. C. Warner, Oxford University Press, 2000.

#### 4. Reference Books:

R1, R2 and R3: Green Catalysis by Paul T Anastas, Wiley, 2010, Vol. 1 Homogeneous catalysis, Vol. 2 Heterogeneous catalysis and Vol. 3 Biocatalysis

### 5. Course Plan:

Lec.	Topics to be covered	Learning Objectives	Reference
No.			(Page no.)
1-3	Introduction, Tools and Principles of Green Chemistry	Definition and overview of the twelve principles of Green Chemistry, E factor and the concept of atom economy, Alternative starting materials, reagents, solvents, product/target molecule process analytical chemistry and catalysts	
4-6	Evaluation of factors for green process	Evaluating effects of: chemistry, feedstock, reaction type, methods to design safer chemicals	T2 5.1- 8.5
7-8	Examples of green chemistry	Polysaccharide polymers, chemical from glucose, halide free synthesis of aromatic amines, alternative to Strecker synthesis, non phosgene isocyanate synthesis, Haas Sea –Nine insecticide	T2 9.1-9.5
9-10	Alternate Energy Sources	Applications of microwave & ultrasound energies in green synthesis	Lecture notes
11-15	The Basics of Catalysis	Homogeneous, heterogeneous and biocatalysis Catalyst Deactivation, Sintering, and Thermal Degradation catalyst Inhibition and Poisoning	Lecture notes







16-18	Solid acids and bases as catalyst	Acidic clays, Zeolites and Zeotypes, Solid Acids Containing Surface SO <sub>3</sub> H Functionality, Heteropoly Acids, Anionic Clays: Hydrotalcites, Basic Zeolites, Organic Bases Attached to Mesoporous Silica	T1 2.1-2.4
19-22	Catalytic reduction	Heterogeneous Reduction Catalysts: General Properties, Transfer Hydrogenation Using Homogeneous and Heterogeneous Catalysts, Chiral Homogeneous and Heterogeneous Reduction Catalysts, Biocatalytic Reductions Enzyme and Whole Cell Technology Technology for Biocatalytic Reduction	T1 3.1-3.5
23-27	Catalytic oxidation	Mechanisms of Metal-catalyzed Oxidations: General Considerations, Homolytic and Heterolytic Mechanisms, Direct Homolytic Oxidation of Organic Substrates, Catalytic Oxygen Transfer, Ligand Design in Oxidation Catalysis, Enzyme Catalyzed Oxidations	T1 4.1-4.5
28-30	Catalytic C–C bond formation	Enzymes for Carbon–Carbon Bond Formation, Transition Metal Catalysis, organocatalysis	T1 5.1-5.4
31-34	Catalysis in Novel Reaction Media	Choice of Solvent, Alternative Reaction Media and Multiphasic Systems, Two Immiscible Organic Solvents Aqueous Biphasic Catalysis, Fluorous Biphasic Catalysis, Supercritical fluids, Ionic liquids	T1 7.1-7.9
35-38	Chemicals from Renewable Raw Materials	Carbohydrates, Chemical and Chemoenzymatic Transformations of Carbohydrates into Fine Chemicals and Chiral Building Blocks, Fats and Oils, Terpenes, Renewable Raw Materials as Catalysts, Green Polymers from Renewable Raw Materials	T1 8.1-8.8
39-42	Cascade and Enantioselective Catalysis	Dynamic Kinetic Resolutions by Enzymes Coupled with Metal Catalysts, Combination of Asymmetric Hydrogenation with Enzymatic Hydrolysis, Catalyst Recovery and Recycling, Immobilization of Enzymes: Cross-linked Enzyme Aggregates, enantioselective catalysis	T1 9.1-9.6

### 6. Evaluation Scheme:

Component	Duration	Weightage	Date Time	Remarks
Mid Semester Test	1.5 hrs.	30%	8/10 8:00 - 9:30 AM	Closed Book
Quiz	continuous	30%		Closed Book
Comprehensive Exam.	3 hrs.	40%	8/12 FN	\$

- \$ The comprehensive examination will have a closed book quiz portion with 15% Weightage, and an open book section with 25% weightage.
- **7. Chamber Consultation Hours:** To be announced through a notice.
- **8. Notices:** Notices, if any, concerning the course will be displayed on the Chemistry Department Notice Board only.
- **9. Make up policy:** Make up would be considered only for genuine reasons.

Instructor in-Charge CHEM F337



