#### DEPARTMENT OF CHEMISTRY

### NATIONAL INSTITUTE OF TECHNOLOGY: TIRUCHIRAPPALLI - 620 015

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# I B.Tech. syllabus for the Board of Studies meeting

### **CHIR 11**

<u>I semester</u> (2 credit theory + 1 credit practical = 3 credit course)

## **Objectives**

To introduce the students to basic principles of chemical bonding, coordination chemistry, reaction mechanism, stereochemical aspects of organic compounds. To provide a brief outline on the types and applications of polymers.

### **Chemical Bonding**

Basic concepts of bonding and applications: VBT, VSEPR theory, MO Theory. Intermolecular interactions-ion ion interactions, ion-dipole interactions, hydrogen bonding, dipole-dipole interactions, London / dispersion forces, relative strength of intermolecular forces; Consequences-surface tension.

## **Coordination and Organometallic Chemistry**

Coordination Chemistry: Crystal field theory, Octahedral, Tetrahedral & Square planar complexes, Jahn-Tellar Distortion, Color, magnetism, EAN Rule, 18 electron Rule, Wilkinson Catalysis, Zieglar-Natta Catalysis, Boranes & Wades rules (the closo-, nido-, arachno- borane structural paradigm, Wade-Mingos and Jemmis electron counting rules) Dioxygen transport and storage-hemoglobin and myoglobin.

## Basic organic reactions and mechanism

Nucleophilic substitution reactions: SN<sup>1</sup>, SN<sup>2</sup>, SN<sup>i</sup> mechanism. Elimination reaction: The E1, E2 and E1cB mechanisms, Hofmann versus Saytzeff elimination, Pyrolytic syn-elimination. Oxidation reaction: with peracids, Pb(OAc)<sub>4</sub>, OsO<sub>4</sub>, SeO<sub>2</sub>. Reduction reactions: reduction with hydride transfer reagents like NaBH<sub>4</sub>, LiAlH<sub>4</sub> and DIBAL-H. Birch reduction.

## **Stereochemistry & Aromaticity**

Representations of three dimensional structures - Types of Isomerism - configurations and chirality, enantiomers, diastereomers, optical activity, absolute configurations and conformational analysis. Applications of chirality in drug molecules. Aromaticity, Huckels rule of aromaticity and anti-aromaticity, annulenes, heteroannulenes.

### **Polymers and Composites**

Concept of macromolecules-Nomenclature of polymers-Tacticity- Polymerization processes-Mechanism-Types of Polymerization-Classification of Polymers-Effect of Polymer structure on properties-Moulding of plastics into articles-Important addition and condensation polymers—synthesis and properties—Molecular mass determination of polymers- Static and dynamic methods, Light scattering and Gel Permeation Chromatography-Rubbers—Vulcanization—Synthetic rubbers—Conducting polymers-Composite materials—Reinforced composites and processing.

#### **Outcome**

Students will learn about the fundamentals and needs of chemical bonding, coordination chemistry, polymers and composites. They will be familiarizing with basics of reaction mechanism and stereochemical aspects of organic molecules.

# **Practicals (Laboratory Experiments):**

- 1. Determination of reaction kinetics of hydrolysis of an ester.
- 2. Estimation of carbonate, non-carbonate and total hardness in the given water sample.
- 3. Percentage purity of bleaching powder.
- 4. Determination of the percentage of Fe in the given steel sample.
- 5. Estimation of Ca in limestone.
- 6. Estimation of Fe<sup>3+</sup> by spectrophotometer.

### **Outcome**

The chemistry laboratory course will consist of experiments illustrating the principles of chemistry relevant to the study of science and engineering. The students will learn to determine the reaction kinetics, estimate various components from corresponding bulk mixture.

### **Reference Books**

- 1. PW Atkins and J de Paula, Physical Chemistry by, Oxford University Press.
- 2. Inorganic Chemistry: Principles of Structure and Reactivity, J E Huheey, E A Keiter, R L Keiter and O K Medhi, 4 th Edn, 2006, Pearson, ISBN: 006042995X.
- 3. Organic Chemistry, Paula Y Bruice, 7th Edition, Springer, 2009, Pearson. ISBN-13: 978-0321819031.