**Inorganic and Physical Chemistry**

1.1 Course Number: CY111
1.2 Contact Hours: 3-1-0 Credits: 11
1.3 Semester-offered: 1st Year-Even
1.4 Prerequisite: Nil
1.5 Syllabus Committee Member: Dr. D. Panda, Dr. Arshad Aijaz, Dr. U. P. Ojha & Dr. A. K. Choubey

**2. Objective:** The objective of the course is to provide an essence of the undergraduate students; molecular orbital theory, CFT, organometallic chemistry, quantum chemistry, phase rules and electrochemistry. The basic understanding of the above subjects will have a bearing in handling some of the engineering courses that the students will undergo in later semesters.

**3. Course Content:**

Unit-wise distribution of content and number of lectures

| Unit | Topics | Sub-topic | Lectures |
|---|---|---|---|
| 1 | Chemical Bonding | Molecular Orbital (MO) Theory, Symmetries in Molecular Orbitals, MO Diagrams of $NH_3$, $H_2O$, $CH_4$, and Metal Complexes | 6 |
| 2 | Transition Metals Chemistry | Crystal Field Theory, Nature of Metal-Ligand Bonding, Stability, Electronic Spectra and Magnetic Properties of Inorganic Complexes | 5 |
| 3 | Organometallic Chemistry | Complexes with Metal-Carbon Sigma Bonds, Metal Carbonyl Complexes, Metal-Alkyl Complexes, Metal Complexes with Pi Acceptor Ligands, Alkene Complexes, Catalysis and Reaction Mechanisms of Metal Complexes | 6 |
| 4 | Quantum Chemistry | Schrodinger equation, Wave functions, Probability density, Operator, Eigen function & Eigen Value Schrödinger Equations, Many electron system Particle in a Box/Ring problem, Hydrogen atom. Atomic orbitals, many electron atoms and spin orbitals | 6 |
| 5 | Electronic Transitions | Implications of discrete energy levels, Population of States – Boltzman Distribution, Interaction of radiation with matter, origin of linewidths in molecular spectra, Transition dipole moment and Fermi's Golden Rule, Potential energy surfaces-Rates of reactions; Steady state approximation and its applications | 5 |
| 6 | Physical Transformation of Substances | Concept of pre-equilibrium; Equilibrium and related thermodynamic quantities. Phase diagrams, The stabilities of phases, Phase boundaries, Three typical phase diagrams, The location of phase boundaries, the | 6 |

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| | | thermodynamic criterion of equilibrium, and the Ehrenfest classification of phase transitions | |
| 7 | Electrochemistry | Nernst equation, Concentration and Formation cells, Equilibrium at Electrode Interface, Double layer, Concept of Polarization, Over Potential, Butler-Volmer and Tafel's equation, Limiting Current Concept, Applications of Electrochemical Kinetics to Fuel Cell, Water Electrolyzer, Batteries and Corrosion | 6 |
| | | **Total** | **40** |

**4.Readings**

4.1 Textbook:

- Physical Chemistry, Atkins, P. W. and de Paula, J., 7th Ed., Oxford University Press.
- Inorganic Chemistry: Shriver and Atkins, Oxford University Press
- Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann, 6th Ed. Wiley
- Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter, 4th Ed. Prentice Hall.
- Electrochemical Methods: Fundamentals and Applications by Allen J. Bard, Larry R. Faulkner

4.2 Reference books:

- General Chemistry, McQuarrie, 4 th Ed., University Science Books.
- Chemistry: A Molecular Approach, Tro, 2nd Ed, Prentice Hall

**5.Outcome of the Course:**

The students will receive an in-depth knowledge in various aspects of Inorganic and Physical Chemistry, and will learn about strategies those shall be adopted to function various metallic compounds. This will aid the aptitude of the students in designing of various inorganic metal-based catalysts targeting various catalytic applications. The course will also provide idea about the quantum chemistry those may be implemented to understand the chemistry at atomic level.