SEMESTER – 1

Paper Name : Inorganic Chemistry (Theory)	**Course Code : CH 401**
Credits : 04	**Learning Hours : 60**

The syllabus encompasses a comprehensive study of various topics in quantum mechanics, inorganic chemistry, and organometallic chemistry. It begins with an exploration of commutation relations, focusing on angular momentum operators, ladder operators, and eigenfunctions of the position operator. Perturbation theory is introduced, covering both first-order and non-degenerate cases, with applications to hydrogen and helium atoms, alongside the variation method's application to the hydrogen atom. Concepts such as tunnelling and the shape of tunnelling barriers are examined. The syllabus delves into organometallic compounds of transition elements, including their stability and diverse ligand types, and their role in catalytic reactions. Crystal field theory, ligand field theory, and molecular orbital theory are explored in detail, along with their applications in understanding d-orbital splitting and complex. Additionally, boranes, inorganic polymers, and organoboron/organosilicon compounds are studied, along with their synthesis, structures, bonding, and applications, providing a comprehensive understanding of advanced topics in chemistry.

By the end of the course, the students will be able to:

- Understand the commutation relations, including angular momentum and ladder operators, and their applications in quantum mechanics.
- Develop proficiency in approximation methods such as perturbation theory and the variation method, and apply them effectively to solve problems related to atomic systems.
- Acquire knowledge of fundamental concepts in tunnelling and barrier shapes, enabling analysis of quantum phenomena in various systems.
- Understand the principles governing organometallic compounds of transition elements, including their stability and catalytic roles in chemical reactions.

- Master crystal field theory, ligand field theory, and molecular orbital theory, and their applications in predicting and interpreting complex structures and electronic configurations.
- Explore the diverse chemistry of boranes, inorganic polymers, organoboron, and organosilicon compounds, including synthesis, structure, bonding, and their significance in organic synthesis and materials science.

DETAILED SYLLABUS

Unit 1 **Quantum Mechanics – I** **(14 Marks)**

- Commutation Relations: Angular Momentum Operators and their commutation relations; Ladder Operators and their commutation relations; Eigen Functions of the position Operator and Dirac Delta function; Projection Operators.
- Approximation method: Perturbation theory (First order and non-degenerate), application to hydrogen and helium atoms; Variation method and application to hydrogen atom.
- The Concept of tunnelling, Shape of the Barriers of tunnelling.

Unit 2 **Organometallic Compounds** **(14 Marks)**

- Organometallic compounds of transition elements, stability of metal carbon bond in complexes
- Synthesis, uses and structure of organometallic compounds of π bonding organic ligands, 2-electron ligands, olifinic and acetylinic complexes, compound with 3 – electrons ligand – allylic complexes, compounds. With 4- electron ligands butadiene complexes, n^4 complexes of cyclopentadiene, compounds with 5 – electrons ligands– cyclopantadionyl, compounds with 6 electron ligands, n^6 complexes of benzene and its derivatives
- Role of organometallic compounds in catalytic reaction complexes of benzene and its derivatives

Unit 3 **Electronic Spectroscopy of Transition metal complexes** **(14 Marks)**

- Concept of crystal field theory (CFT), ligand field theory (LFT) and molecular orbital theory (MOT).
- Splitting of d-orbitals in various stereochemistry; tetragonal distortion in octahedral complexes.
- Spectrochemical series; nephelauxetic series; electronic states and term symbols.

Unit 4 **Symmetry (Group Theory) (14 Marks)**

- **Matrices, Vectors and Operators:** Matrix Algebra, Mathematics of matrices, Vectors, Eigen values and Eigen vectors, Transformation Operators,
- **Representation of point groups:** Unit vectors as the basis for representation, Rotational vectors as the basis for representation, Position vectors as the basis for representation, Wave functions as the basis for representation, Construction of character table of point group C_{2v} and C_{3v} .
- **Reducible and irreducible representations:** Generated by bond vectors and by various orbitals
- **Great Orthogonality Theorem and Character Table:** GOT, General rules derived from GOT, Relation between reducible and irreducible representations of a point group, criteria for irreducibility, Construction of character table and notations followed, direct product representations

References

1. Advanced Inorganic Chemistry, By: Cotton, Wilkinson, Murillo and Bochmann (1999).
2. Organometallic Chemistry a Unified Approach by R.C.Mehrotra and A.Singh.
3. Organometallic Chemistry of Transition Metals by Robert H.Crabtree.
4. Introductory Quantum Chemistry, Fourth Edition, By: A. K. Chandra Tata McGraw-Hill Publishing Company Ltd., New Delhi (1994).
5. Inorganic Chemistry, Shriver and Atkins, Oxford University Press.
6. Inorganic Chemistry, James E. Huheey, Eilen A. Keiter, Richard L. Keiter, Pearson Education.
7. Group theory and symmetry in chemistry, L. H. Hall (McGraw Hill)
8. Group theory in Chemistry V. Ramkrishnan & M. S. Gopinadhan Vishal Pub.1996.