BACHELORS WITH CHEMISTRY AS MAJOR
5th SEMESTER
CHM522J3: CHEMISTRY _ ADVANCED INORGANIC CHEMISTRY

CREDITS: THEORY-4, TUTORIALS-2

THEORY (4 CREDITS: 60 HOURS)

Course Objectives: *To provide exposure of various biomolecules containing metal ions that comprises many important enzymes and proteins and fundamental understanding of organometallic compounds and pi-acid complexes. Furthermore, students will have a basic understanding of Molecular symmetry.*

Learning outcomes:
After completing this course, the student is expected to learn the following

- *Importance of metal ions in biology and knowledge of various enzymes and their activities*
- *Advanced applications of bioinorganic chemistry in the field of medicine.*
- *Basic understanding of organometallic compounds, preparation, properties and structural analysis of pi-acid complexes*
- *Knowledge of molecular symmetry and point groups.*

Unit-I Biological Inorganic Chemistry (15 hours)

Metalloenzymes: Structure, mechanism of action: Carbonicanhydrase, carboxypeptidase and Nitrogenase. Biological chemistry of Molybednum (Xanthine oxidase) and cobalt (Vit B12). Structure and biological role of Rubredoxin and Ferridoxin, Blue Copper proteins: (Oxidases and Plastocyanin). Cytochrome P450.
Therapeutic applications of cis-platin, transition metal radio-isotopes (Tc)and MRI (Gd) agents. Toxicity of metals and chelation therapy (Therapeutic aspects of chelating drugs: conditional stability constant, HSAB theory).

Unit –II Organometallic Chemistry: (15 hours)

Definition and classification of organometallic compounds. hapticity concept, Applications of 18-electron rule. Stability of organometallic compounds. Decomposition pathways (Beta elimination reaction). Comparison of main group and transition metal organometallic compounds. Preparation, structure and bonding in Zeise's salt. Homogenous and heterogenous catalysis, catalytic efficiency: TON and TOF. Mechanism of Alkene hydrogenation and Hydroformylation reactions using transition metal catalysts.

Unit-III: pi-acid Complexes of Transition Metals: (15 hours)

Transition Metal Carbonyls: Carbon Monoxide as ligand; synthesis, reactions and bonding in mononuclear carbonyls (synergistic bonding). Selected EAN examples of poly-nuclear metal carbonyls. Spectral analysis of metal carbonyl compound (FTIR). Preparation and binding modes of transition metal Nitrosyls and Dinitrogen complexes. Tertiary phosphine as ligand.

Unit IV: Molecular Symmetry (15 hours)

Molecular Symmetry - Symmetry elements and operations. Identity. Proper axis of rotation, order of axis, and principal axis. Reflection plane: horizontal, vertical and dihedral planes. Inversion centre. Improper axis of rotation. Combination of symmetry operations-General considerations, group multiplication tables. Symmetry subgroups and classes. Mathematical requirements of a group. Point groups-Schoenflies notation of point groups.

BOOKS RECOMMENDED

1. Coordination Chemistry; Banerjee, D.; Tata Mc Graw Hill; 1997.
2. Concise Coordination Chemistry; Gopalan, R. & Ramalingam, V.; Vikas; 2003.
3. The Biological Chemistry of Elements; Frausto de Silva, J.J. R. & Williams, R.J.P.; Oxford; 1994.
4. Bio-inorganic Chemistry of Elements; Hussain Reddy, K.; New Age; 2005.
5. Chemical Applications of Group Theory; 2nd edn.; F. A. Cotton; Wiley Eastern; (1994)
6. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.
7. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.
8. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E. Huheey, Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc.
9. Inorganic chemistry (5th ed.) by Catherine E. Housecroft & Alan G. Sharpe, Prentice Hall, Pearson.

TUTORIALS (2 CREDITS: 60 HOURS)

- Basics of computer-aided drug design (CADD), 3D visualization of Biotargets using free software's. Hands on with drawings of chemical structures of small molecules, Demonstration of Molecular Docking experiment with basic data analysis using free software (AutoDock).
- Hands-on with molecular models for identification of the symmetry elements and point groups.
- Utilization of online resources like Symmetry@otterbein [Symmetry@Otterbein - Symmetry Tutorial (symotter.org)], for better apprehension.