*Title: Coordination Chemistry*

**Objectives:** The major objectives of this course are: (a) To understand the key features of coordination compounds, including the variety of structures, oxidation numbers and electronic configurations, coordination numbers, ligands, chelates, bonding and stability of complexes. (b) To be able to describe the stability of metal complexes and to become familiar with some applications of coordination compounds.

**Outcomes:** After completing this course the students are able to:

1. Understand the coordination numbers, stability and geometric shapes of the complexes
2. Study and compare between the various theories of coordination
3. Explain the reaction mechanisms of coordination compounds

**Course Code:** CH-807

**Credit Hours:** 3-0

**Course Contents:**

1. Introduction to transition metals
2. Historical development of coordination compounds and Werner Theory
3. IUPAC nomenclature of complexes
4. Coordination number (CN) and geometry (shape) of complexes (CN 2-6)
5. Isomerism and classification of isomers
6. Bonding Theories
7. Crystal Field Theory (CFT)
8. Molecular Orbital Theory (MOT)
9. d-d spectrum theory
10. Kinetic and Mechanism
11. **Reactions of Coordination Compounds –**Stabilization of complexes
12. Application of coordination compounds

**Course Contents with proposed contact Hours (Weekly plan):**

**Lecture wise Breakdown**

| W#1 | Topics | Lect # |
|---|---|---|
| 1 | Introduction to Transition Metals | 1 |
| | Lab-1: Introduction to Computational Methods<br>Software Installation – SuperComputer Accounts | 2-3 |
| 2 | Historical development of coordination compounds and Werner Theory<br>Isomerism and classification of isomers | 4 |
| | Lab-2: Tutorial -1 | 5-6 |
| 3 | IUPAC nomenclature of complexes | 7 |
| | Lab-3: Tutorial – 2<br>Group Discussion about the Research Project for this Course | 8-9 |
| 4 | Coordination number (CN) and geometry (shape) of complexes (CN 2-6) | 10 |

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| | Lab-4: Tutorial – 3<br>Finalization of Research Projects<br>**ASSIGNMENT – 1:** Term Paper – Review article (seminal paper - publication last 5 to 10 years) on (any) topic of Coordination Complexes/ Compounds (Your Choice) to be submitted in 02 phases. Phase – 1: Abstract Submission within 02 weeks, Phase –II: Review article submission within 02 months. | 11-12 |
| 5 | | 13 |
| | Lab -5: Model Geometries of Coordination Compounds/Complexes | 14-15 |
| 6 | Bonding Theories:<br>a. VBT<br>b. Hybridization | 16 |
| | Lab-6: Geometry Optimization | 17-18 |
| 7 | Crystal Field Theory | 19 |
| | Lab-7: **Assignment-2:** Independent work on the Geometry modeling and Optimization | 20-21 |
| 8 | Revision of all topics till date | 22 |
| | Assignment-2: Result Submission | 23-24 |
| 9 | **Mid Semester Exam** | 25-27 |
| 10 | Molecular Orbital Theory | 28 |
| | Lab-8: Frequency Calculations for Validation | 29-30 |
| 11 | d-d Spectrum Theory/ Electronic Spectra | 31 |
| | Lab-9: Single Point Energy Calculations | 32-33 |
| 12 | d-d Spectrum Theory/ Electronic Spectra | 34 |
| | Revision<br>Submission of "**Introduction"** section on the Coordination Compounds selected for study | 35-36 |
| 13 | Kinetics and Mechanism | 37 |
| | Lab-10: Natural Bond Order Calculations<br>Submission of "**Methodology "** section on the Coordination Compounds selected for study | 38-39 |
| 14 | Reaction and Catalysis | 40 |
| | Lab-11: Data Compilation | 41-42 |
| 15 | Reactions of Coordination Compounds – Stabilization of complexes | 43 |
| | Lab-12: Data Validation | 44-45 |
| 16 | Application of Coordination Compounds | 46 |
| | Lab-13: Project Report Submission | 47-48 |
| 17 | Presentations + Revision + Problem Solving<br>Assignment-1: Paper Submission | 49-51 |
| 18 | **End Term** ☺ | 52-54 |

**Details of lab work/workshop practice, if applicable:**

Lab sessions will mainly focus on the hands-on training in connection with the lectures taught in class. Details are mention in the week wise breakdown.

**Recommended reading, including textbooks, reference books with dates**

**1.** Bridget Kent, "Advanced Inorganic Chemistry", NY Research Press, **2019**

2. Robert Crabtree, The Organometallic Chemistry of the Transition Metals, 7th Edition, Wiley & Sons In, **2019**.
3. D. Shriver and P. Atkins, Inorganic Chemistry, 5th Edition. Oxford University Press, **2010**.
4. Gary L. Miessler and Donald A Tarr, *Inorganic Chemistry*, 4th Edition, Pearson Prentice Hall, **2010**.
5. "Encyclopedia of Computational Chemistry", 5th volume, John Wiley and Sons, Inc. 1998.
6. Relevant Publications

**Nature of Assessments**

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|---|---|
| Homework/ Assignments: | 5% |
| Quizzes: | 5% |
| MSE: | 30% |
| Final Exam: | 40% |
| Project: | 20% |