



**Department of Chemistry**

**College of Science**

**University of Salahaddine**

**Subject: Inorganic Chemistry (coordination compounds)**

**Course Book – 3<sup>rd</sup> Stage-2<sup>nd</sup> course**

**Lecturer's names: M.Sc. Muhammad Haji Khalil**

**Academic Year: 2023/2024**

# Course Book

1. Course name	Theoretical inorganic chemistry (coordination compounds)
2. Lecturer in charge	Muhammad Haji Khalil
3. Department/ College	Chemistry/science
4. Contact	<a href="mailto:muhamma.khalil@su.edu.krd">muhamma.khalil@su.edu.krd</a> <a href="mailto:muhammed.haji@ymail.com">muhammed.haji@ymail.com</a>
5. Time (in hours) per week	Theoretical: 3
6. Office hours	Tuesday 9:30-11:30 am
7. Course code	
8. Teacher's academic profile	Obtained B.Sc. in 1999, M.Sc. in 2011
9. Keywords	Inorganic chemistry, transition metals, ligands and coordination compounds.
<p><b>10. Course overview:</b> <b>What is Inorganic Chemistry?</b></p> <p>With this lesson, you will learn the definition of inorganic chemistry. You will also learn the types of inorganic compounds, how they react and their applications in several industry sectors.</p> <p><b>Inorganic chemistry</b> is the study of the <i>formation, synthesis and properties</i> of compounds that do not contain carbon-hydrogen bonds. Chemical substances containing carbon-hydrogen bonds are studied in <b>organic chemistry</b>.</p> <p><b>Importance of chemistry in our daily life:</b></p> <p>The importance of chemistry in daily life is that the elements studied in chemistry are the elements that make up the entire world; everything we touch and see and can sense. The importance of chemistry in daily life is that the elements studied in chemistry are the elements that make up the entire world; everything we touch and see and can sense is a result of chemistry. Because this is true, it is important that we understand how these elements compounds came to be, what they can do, and how they work together, so that we can build upon our knowledge, make new discoveries, and change the way our world comes together.</p> <p>Inorganic chemistry is concerned with the properties and behavior of inorganic compounds, which include metals, minerals, and organometallic compounds. While organic chemistry is defined as the study of carbon-containing compounds and inorganic chemistry is the study of the remaining subset of compounds other than organic compounds, there is overlap between the two fields (such as organometallic compounds, which usually contain a metal or metalloid bonded directly to carbon).</p>	
<p><b>11. Course objective:</b></p> <p>This course includes a detailed overview of coordination chemistry, hypothesis and theories which proposed for interpreting the nature of coordinating bonds between metal ions and ligands, such as VBT, CFT and MOT,</p> <p>The principles governing metal—ligand complex stability and specificity depend on the properties of both the metal ion and the chelating agent, as summarized briefly in the following sections. More comprehensive reviews on ligand design for selective complexation of metal ions in aqueous solution are available. This discussion sets the stage for understanding the properties of the compounds presented throughout this article.</p> <p>1.They are used in photography, i.e., AgBr forms a soluble complex with sodium thiosulfate in photography. 2.K[Ag(CN)<sub>2</sub>] is used for electroplating of silver, and K[Au(CN)<sub>2</sub>] is used for gold plating.</p>	

3. Some ligands oxidize  $\text{Co}^{2+}$  to  $\text{Co}^{3+}$  ion.
4. Ethylenediaminetetraacetic acid (EDTA) is used for estimation of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  in hard water.
5. Silver and gold are extracted by treating zinc with their cyanide complexes.

### **12. Student's obligation**

the attendance & completion of all tests assignments and Quiz

### **Syllabus of Coordination Chemistry**

2 Hours/week (theory) + (practice) 3 hours/week

### **Practical:**

#### **Quizzes**

In class every week, the students should already have knowledge of subject that they had taken before, and ready for any quizzes.

Reports and Seminar exams

### **13. Forms of teaching**

White Board and data show

### **14. Assessment scheme**

Breakdown of overall assessment and examination

The students are required to do two closed examinations at the course besides other assignments, for example daily quizzes and other activities which may hold 5% of total grades (5 marks), final examination which bears 50% from the total degrees. Over all degrees 15% theory (2 hours per week) and 35% practical (3 hours per week).

The student are required to achieve one closed exam at the mid of each semester for practical course beside other assignments. For each experiment the students must prepare full text paper which includes theory, calculations, discussion and homework.

The grades are arranged as follows:

Semester exam: 10 %

Class room and assignments 2 %

Absence and Quiz: 3 %

It means 15% for each semester.

### **15. Student learning outcome:**

Preparation complexes and determination their contents and absorbances.

#### **“Medicinal Applications of Coordination Chemistry”**

Inorganic compounds have been used in medicine for thousands of years, often without a known molecular basis for their mechanism of action, and with little attempt to design them. The design of coordination (metal) complexes is not an easy task. The organic chemist often deals with diamagnetic compounds which are both kinetically and thermodynamically stable, and benefits from the use of well developed speciation techniques, especially  $^1\text{H}$  and  $^{13}\text{C}$  nuclear magnetic resonance (NMR) spectroscopy. For metal compounds the situation is more complicated. Ligand substitution and redox reactions can be facile, can occur over very wide timescales, and are not so easily followed by conventional techniques, especially under

physiologically relevant conditions (for instance, at micro molar concentrations). But the challenge is real and worth exploring. We need new drugs with novel mechanisms of action. Inorganic chemistry offers that possibility.

### **Platinum Anticancer Drugs**

Two areas of work have highlighted the potential of inorganic chemistry in recent years: the platinum anticancer field and gadolinium compounds, used as contrast agents in magnetic resonance imaging (MRI). Both of these are well covered in this new book. Platinum commands about forty pages. This is warranted. Platinum compounds are now the world's best-selling anticancer drugs – they have billion-dollar sales each year. If you are not familiar with atomic structure, types of chemical bonds, oxidation states, coordination geometries, isomerism, electronic structure and magnetism, then there are some one hundred pages (just over a quarter of the book) of introduction to help you, including the background on square-planar platinum complexes needed to understand the mechanism of action of the first platinum complex to be approved for clinical use: cisplatin (*cis*-diamminedichloroplatinum (II)).

Inorganic compounds are used as catalysts, pigments, coatings, surfactants, medicines, fuels, and more. They often have high melting points and specific high or low electrical conductivity properties, which make them useful for specific purposes.

## **:16. Course Reading List and References**

1. S. Z. Haider, *Advanced Inorganic Chemistry*.
2. James E. Huheey, *Inorganic Chemistry*.
3. Cotton, Wilkinson and Gaus, *Basic Inorganic Chemistry*.
4. Shriver, Atkins and Langford, *Inorganic Chemistry*.
5. Douglas. McDaniel and Alexander, *Concepts and Models of Inorganic Chemistry*.
6. Sharpe, *Inorganic Chemistry*.
7. W. L. Jolly, *Inorganic Chemistry*.
8. Purcell and Kotz: *Advanced Inorganic Chemistry*
9. J. E. Huheey: *Inorganic Chemistry*
10. J. D. Lee: *Inorganic Chemistry*
11. M.L. Tobe: *Inorganic Reaction Mechanism*
12. Shriver, Atkins and Langford: *Inorganic Chemistry*

13. Douglas, McDaniel and Alexander: Concepts and Models of Inorganic Chemistry

14. Katakis and Gordon: Mechanism of Inorganic Reactions

**17. The Topics:**

**Lecturer's name**

**An Introduction to Coordination chemistry: (4 weeks)**

**Muhammad Haji Khalil**

**Bonding Theories for Coordination Compounds:**

**(Crystal Field Theory (CFT): ( 7weeks).**

Shapes of 3d orbitals

Degenerate of d-orbitals, properties, splitting of d-orbitals in different fields:  
Octahedral (O.h), square planar (sq.pl.) and Tetrahedral (T.H) fields.

Crystal Field Stabilization Energy (CFSE):

Magnetic Measurements, High-spin and low-spin, Strong field and weak field.  
Crystal field stabilization energy, high spin and low spin complexes, Pairing energies, factors affecting the magnitude of CF splitting energies.  
Spectrochemical series, Jahn-Teller effects, limitations of Jahn-Teller theory.

**Molecular orbital theory: (3 weeks):**

Linear combination of atomic orbitals (LCAO):

s, p and d orbital overlaps:

Basic principle,  $\sigma$  -bonding and  $\pi$  -bonding in octahedral complexes,  
effects of  $\pi$  -bonding on stability of the complexes.

MOT in tetrahedral and octahedral complexes, limitations of MOT, comparison of different approaches to bonding in coordination compounds.

18. Practical Topics	Lecturer's name
<p>Introduction of Practical inorganic chemistry</p> <p>1-Preparation of tetraamminecopper(II)sulphatehydrate <math>[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}</math> .</p> <p>2-Preparation of bis(acetylacetonato) copper(II) <math>[\text{Cu}(\text{acac})_2]</math>.</p> <p>3-preparation of trans-bis(acetylacetonato) diaquanickel(II), <math>[\text{Ni}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]</math>.</p> <p>4-Preparation of bis(acetylacetonato) diaquacobalt(II) <math>[\text{Co}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]</math></p> <p>5-Preparation of trans-bis (acetylacetonato) diaqua Manganes(II), <math>[\text{Mn}(\text{C}_5\text{H}_7\text{O}_2)_2(\text{H}_2\text{O})_2]</math></p> <p>6- Preparation of Cis-potassium diaquabis(oxalato)chromate(III) dihydrate <math>\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}</math>.</p> <p>7- Determination of <math>\text{C}_2\text{O}_4^{2-}</math> in the complex <math>\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}</math>.</p> <p>8- Determination of <math>\text{Cr}^{3+}</math> in the complex <math>\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}</math>.</p> <p><b>References :</b></p> <ol style="list-style-type: none"> <li>1. Inorganic Experiments by J.Derek Woollins.</li> <li>2. Inorganic Chemistry by Shriver and Atkins.</li> <li>3. Inorganic Chemistry by Carthrine E. Housecroft.</li> <li>4. Basic Inorganic Chemistry by Cotton and Wilkinson.</li> <li>5. Modern Inorganic Chemistry by Jolly.</li> <li>6. Modern Inorganic Chemistry by Lagowski.</li> </ol>	<p>Lecturer names: Muhammad Haji Khalil &amp; Adnan Muhammad Qdir (3hrs)</p> <p>22/1/2023</p> <p>29/1/2023</p> <p>6/2/2023</p> <p>....</p> <p>.....</p> <p>.....</p> <p>....</p> <p>.....</p>
<p>Q1/ Between <math>[\text{Mn}(\text{CN})_6]^{3-}</math> and <math>[\text{Mn}(\text{CN})_6]^{4-}</math> , <math>[\text{Co}(\text{CN})_6]^{3-}</math> and <math>[\text{CoF}_6]^{3-}</math>, <math>[\text{NiCl}_4]^{2-}</math> and <math>[\text{PdCl}_4]^{2-}</math>, <math>[\text{Cu}(\text{NH}_3)_6]^{2+}</math> and <math>[\text{Cr}(\text{NH}_3)_6]^{2+}</math> Which is more likely to be high spin? Why? At.No. Mn=25, Co=27, Ni=28, Pd=47, Cu=29, Cr=24.</p> <p>Q2/ For the <math>[\text{Cr}(\text{H}_2\text{O})_6]^{2+}</math> ion the main pairing energy P is found to be 23500 <math>\text{cm}^{-1}</math>. The magnitude of <math>\Delta_o</math> 13900 <math>\text{cm}^{-1}</math>. Calculate the CFSE for the complex in configurations corresponding to high spin or low spin states , which is more stable? <math>_{24}\text{Cr}</math></p> <p>Q3/a) using CFT, depict the electronic of the Rhodium(II)ion in an O.h field for which the CFS <math>\Delta_o</math> is less than the pairing energy P. b) calculate the CFSE for the configuration in terms of <math>\Delta_o</math> and P . <math>_{45}\text{Rh}</math></p> <p>Q4/ determine the CFSE of <math>d^6</math> complex having <math>\Delta_o = 25000 \text{ cm}^{-1}</math> and <math>P = 15000 \text{ cm}^{-1}</math></p> <p>Q5/ Determine the configuration (in the form <math>t_2g^m e_g^n</math> or <math>e_g^m t_2g^n</math>, as appropriate), the number of unpaired electrons, and the ligand field stabilization energy as a multiple of <math>\Delta_o</math> or <math>\Delta_T</math> for each of the following complexes using the spectrochemical series to decide, where relevant, which are likely to be strong-field and which weak-field.</p>	

(a)  $[\text{Co}(\text{NH}_3)_6]^{3+}$ ; (b)  $[\text{Fe}(\text{OH}_2)_6]^{2+}$ ; (c)  $[\text{Fe}(\text{CN})_6]^{3-}$ ; (d)  $[\text{Cr}(\text{NH}_3)_6]^{3+}$ ; (e)  $[\text{W}(\text{CO})_6]$ ; (f)  $[\text{FeCl}_4]^{2-}$  and (g)  $[\text{Ni}(\text{CO})_4]$ .

Q6/calculate the CFSE for  $[\text{Co}(\text{NH}_3)_6]^{3+}$ , the pairing energy =  $19150 \text{ cm}^{-1}$ , and the  $\Delta$  magnitude =  $23000 \text{ cm}^{-1}$ ,  $C_0 = 27$ .

Q7/calculate CFSE  $[\text{Cr}(\text{en})_3]^{3+}$   $\Delta = 21900 \text{ cm}^{-1}$ .

Q8/calculate the CFSE for  $[\text{FeBr}_4]^{2-}$  At.no. Fe=26.

Q9/calculate the CFSE for electronic configuration  $e_4t_{2g}$ .

Q10/ Draw the crystal field splitting for the following complexes:

$[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$  and  $[\text{Cr}(\text{NH}_3)_6]^{3+}$ .

Q11/ what color expected for complex that absorbs light at  $600 \text{ nm}$ ?

Q12/ what color expected for an octahedral complex appears if energy  $\Delta_0 = 3.75 \times 10^{-19} \text{ J}$ , Plank const. =  $6.626 \times 10^{-34} \text{ J}\cdot\text{s}$ , speed light =  $3 \times 10^8 \text{ m/s}$ .

Q13/ Would you expect a violet solution to be high spin or low spin? What about a red solution?

Q14/ there are two solutions, one which is yellow and another is violet. The solutions are  $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$  and  $[\text{Cr}(\text{CN})_6]^{3-}$  what are the colors of each solution?

Q15/ for which member of the following pairs of complexes would  $\Delta_0$  be the larger and why?

$[\text{CrF}_6]^{3-}$  and  $[\text{Cr}(\text{NH}_3)_6]^{3+}$

$[\text{Fe}(\text{CN})_6]^{4-}$  and  $[\text{Fe}(\text{CN})_6]^{3-}$

Q16/ A-Between  $[\text{NiCl}_6]^{4-}$  and  $[\text{NiCl}_4]^{2-}$  Which one is more likely to be high spin and weakly field? Why? Then calculate CFSE for it if you know  $\Delta_0 = 13900 \text{ cm}^{-1}$  and  $P = 18000 \text{ cm}^{-1}$  and the color of it from dark or light? Explain.

At.No. Ni=28.

B- Draw CFT diagram to show electrostatic force between metal ion and donor atom.

## 20. Extra notes:

Here the lecturer shall write any note or comment that is not covered in this template and he/she wishes to enrich the course book with his/her valuable remarks.

## 21. Peer review :

This course book has to be reviewed and signed by a peer. The peer approves the contents of your course book by writing few sentences in this section.

*(A peer is person who has enough knowledge about the subject you are teaching; he/she has to be a professor, assistant professor, a lecturer or an expert in the field of your subject).*