Republic of Iraq
Ministry of Higher Education & Scientific research
Al-Mustaqbal University
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Introduction in Chemistry

For

First Year Student/course 2

Lecture 7

By

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Method of Writing a Complex Compound

1. The complex consists of a (central atom), typically a metal, which carries the primary valence (the oxidation state of the metal, which can be positive, negative, or neutral, i.e., zero).

2. The metal is surrounded by a group of (ligands) (charged or neutral). These ligands are coordinated to the metal through coordinate bonds, forming a structure known as the coordination sphere.

3. The resulting group, composed of the metal and its ligands, is enclosed within square brackets [ ] and is referred to as the coordination complex.

4. The coordination complex carries a charge if the net charge of the metal and ligands is greater or less than zero. In this case, it is called a complex ion.

5. If the net charge of the complex equals zero, this means the complex does not dissociate in water and is called a neutral complex.

6. A coordination compound may consist of either:

- positively charged complex ion and a simple negative ion, or
- negatively charged complex ion and a simple positive ion.

7. The simple negative or positive ion is located outside the coordination sphere.

Lewis acids: An atom or molecule that possesses an empty orbital capable of accepting an electron pair. In coordination complexes, the metal acts as a Lewis acid.

Lewis bases: An atom or molecule that possesses an electron pair capable of participating in the formation of a coordinate bond. The ligands are considered Lewis bases.

Coordinate bond:

It is the bond that forms between two atoms, where one atom has a **shareable electron pair** and the other has an **empty orbital** to receive this electron pair.

Ligand: A molecule or ion that binds to the central atom (the metal) through coordinate bonds by donating electron pairs to the metal that forms the coordination complex. The ligand may donate:

- A single electron pair (called monodentate)
- Two electron pairs (called bidentate)
- Or more electron pairs

The Central Ion: Coordination compounds are characterized by having a central atom that receives electron pairs, typically a metal that forms coordinate bonds with ligands. This central atom is called the **central ion**, which may carry a positive, negative, or neutral charge, known as the **primary valence**. When the central atom exhibits a charge, it is then referred to as the **central ion**.

Coordination Complex:

A compound formed by the union of a central atom (metal) with several ligands through coordinate bonds.

Oxidation Number:

The charge carried by the metal in the coordination complex, which may be negative, positive, or zero.

Example: Calculate the charge of the central atom in the complex- $[Co(NH_3)_5Cl]Cl_2$

Solution: When a complex consists of both positive and negative components (i.e., is not an ion), the total net charge equals zero, as in our example above.

$[Co(NH3)_5Cl]\ Cl_2$

X + 5(0) + (-1) + 2(-1) = 0

X + 0 -1-3 = 0 X= +3 the coordination number of cobalt CO^{+3}

Example: Calculate the charge of the central atom in the complex- $[Cr(en)(NH_3)_2 I_2]^+$

$[Cr(en)(NH_3)_2I_2]^+$

X + 0 + 2(0) + 2(-1) = +1

X + 0-2 =+1 X = +3 the coordination number of chromium Cr^{+3}

Coordination Number:

The number of molecules or ions attached to the central atom, multiplied by the number of donor sites (denticity) the ligand possesses—or alternatively, the total number of direct bonds formed with the central atom. It can generally be calculated by counting the electron pairs surrounding the central atom, represented as straight lines between the central atom and the ligand's donor sites.

Coordination number = (Total molecules/ions within the coordination sphere) $[Co(NH_3)_5Cl]Cl_2$

6= 1+5

Complex Ion: An ion consisting of a central atom or ion surrounded by ligands, where the coordination sphere exhibits either a positive or negative net charge resulting from the combined charges of the metal and ligands.

Example Calculation for $[Fe(CN)_6]^{4-}$:

- Each cyanide (CN^-) ligand carries a charge of -1
- For 6 ligands: 6 × (-1) = -6
- Iron (Fe) has a charge of +2.
- Net charge: +2 + (-6) = **-4** → Thus, the complex ion is **$[Fe(CN)_6]^{4-}$**.

Neutral Complex:

A complex formed when the central atom/ion and surrounding ligands result in a net charge of zero within the coordination sphere.

$[Pt^{2+}(NH3)_2 Cl_2]$

Net charge: +2 + 0 + 2(-1) = 0

Effective Atomic Number (EAN) Rule:

This rule states that a coordination complex becomes stable when the total number of electrons on the metal (including those donated by ligands) equals the atomic number of a noble gas (e.g., Kr [36], Xe [54], or Rn [86]).

Key Formula:

EAN = (Metal's atomic number) + (Electrons donated by ligands)

Q1:Does the effective atomic number rule apply to this compound?

1. **Oxidation state calculation:**

    - Pd: x + 6(0) = +4 → **x = +4**
    - Atomic number of Pd = **46**

2.Remaining electrons on Pd: 46 (Pd) - 4 (lost e^-) = **42 electrons**

3.Electrons donated by ligands:

- Each NH_3 donates **2 electrons** (lone pair).
- 6 NH_3 ligands → 6 × 2 = **12 electrons**

4.Total EAN: 42 (Pd remaining e^-) + 12 (from ligands) = **54**

54 = Atomic number of Xe (Xenon) → Rule applies!

Q2: Explain whether the atomic number rule applies to the compound **$[Ni(en)_3]^{+2}$** ?

1. **Determining Nickel's Oxidation State:**

- Total complex charge = +2
- Ethylenediamine (en) is neutral
- Thus: x + 3(0) = +2 → **Oxidation state (x) = +2**

2. **Nickel's Atomic Number = 28**

2. Calculating Remaining Electrons on Nickel: 28 (atomic number) - 2 (lost electrons) = **26 electrons**

3. **Electrons Donated by Ligands:**

- Each en donates 4 electrons (bidentate)

- 3 en × 4 electrons each = **12 electrons**

4. **Effective Atomic Number (EAN):**

- 26 (remaining Ni electrons) + 12 (from ligands) = **38**

5. **Comparison with Noble Gases:**

- Doesn't match any noble gas atomic numbers (36-Kr, 54-Xe, 86-Rn)

Final Result:

The EAN rule **does not apply** to $[Ni(en)_3]^{2+}$ because the EAN (38) doesn't equal any noble gas configuration.

Analysis of the Effective Atomic Number (EAN) Rule for $[Ni(CO)_4]$:

1) Determining Nickel's Oxidation State:

- Total complex charge = 0 (neutral)
- CO is neutral
- Thus: x + 4(0) = 0 → **Oxidation state (x) = 0

2) Nickel's Atomic Number = 28

3) Calculating Remaining Electrons on Nickel:

- 28 (atomic number) - 0 (no electrons lost) =28 electrons

4) Electrons Donated by Ligands:

- Each CO donates 2 electrons
- 4 CO × 2 electrons each = 8 electrons

5) Effective Atomic Number (EAN):

- 28 (Ni electrons) + 8 (from ligands) = 36

6) Comparison with Noble Gases:

- Perfect match with Krypton (Kr) atomic number (36)

Final Result:

The EAN rule fully applies to $[Ni(CO)_4]$ as it achieves the stable noble gas configuration of Krypton (36).

Analysis of the Effective Atomic Number (EAN) Rule for $[Co(NO_2)_6]^{3-}$:

1. **Determining Cobalt's Oxidation State:**
    - Total complex charge = -3
    - Each NO_2^- ligand has -1 charge
    - Thus: x + 6(-1) = -3 → x - 6 = -3 → **Oxidation state (x) = +3**
2. **Cobalt's Atomic Number = 27**
3. **Calculating Remaining Electrons on Cobalt:**
    - 27 (atomic number) - 3 (lost electrons) = **24 electrons**
4. **Electrons Donated by Ligands:**
    - Each NO_2^- donates 2 electrons (nitrito ligand through N)
    - 6 NO_2^- × 2 electrons each = **12 electrons**
5. **Effective Atomic Number (EAN):**

- 24 (remaining Co electrons) + 12 (from ligands) = **36**

6. **Comparison with Noble Gases:**
    - Perfect match with Krypton (Kr) atomic number (36)

Final Result:
The EAN rule **applies perfectly** to $[Co(NO_2)_6]^{3-}$ as it achieves the stable noble gas configuration of Krypton (36).

Analysis of the Effective Atomic Number (EAN) Rule for $[Ag(NH_3)_4]^+$:

1. **Determining Silver's Oxidation State:**
    - Total complex charge = +1
    - NH_3 is neutral
    - Thus: x + 4(0) = +1 → **Oxidation state (x) = +1**
2. **Silver's Atomic Number = 47**
3. **Calculating Remaining Electrons on Silver:**
    - 47 (atomic number) - 1 (lost electron) = **46 electrons**
4. **Electrons Donated by Ligands:**

- Each NH_3 donates 2 electrons
- 4 NH_3 × 2 electrons each = 8 electrons

5. Effective Atomic Number (EAN):

- 46 (remaining Ag electrons) + 8 (from ligands) = 54

6. Comparison with Noble Gases:

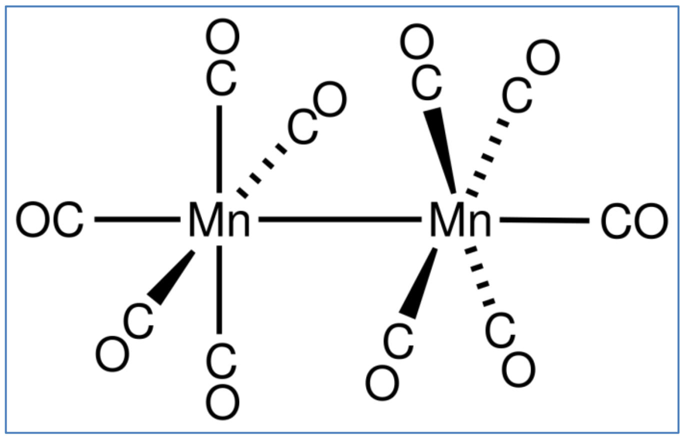
- Perfect match with Xenon (Xe) atomic number (54)

Final Result:

The EAN rule applies perfectly to $[Ag(NH_3)_4]^+$ as it achieves the stable noble gas configuration of Xenon (54).

This theory applies to all carbonyl complexes where the central atom has an **odd atomic number**. It has been found that such complexes do not exist as **dimeric molecules**."

$[Mn_2(CO)_{10}]$

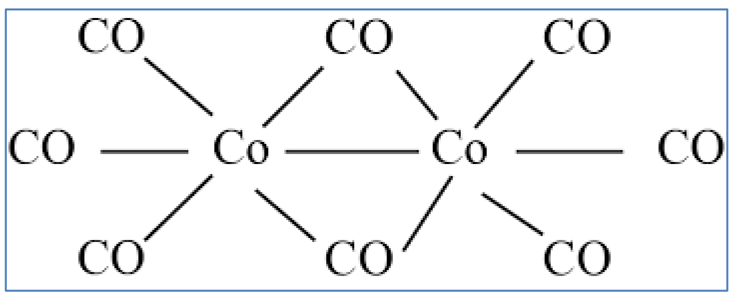


Mn = 25   Mn-Mn = 1e

5CO = 5x2 = 10 e

25 + 1 + 10 = 36= Kr =EAN

[$Co_2(CO)_8$]



Co = 27e   Co – Co = 1 e

4Co =4x2= 8

27 + 1 + 8 = 36= Kr =EAN

Magnetic properties

The Role of Magnetic Properties in Coordination Complexes:

The magnetic properties of complexes play a crucial role in explaining bonding theories (chemical compound formation). These properties arise from two distinct electron configurations:

1. **Unpaired Electrons (↑):**
   - Results in **paramagnetic** behavior.
   - Paramagnetic materials are **attracted** to an external magnetic field and align with it, exhibiting significant magnetic effects.
   - The **strength of attraction** depends on the number of unpaired electrons.
2. **Paired Electrons (↑↓):**
   - Results in **diamagnetic** behavior.
   - Diamagnetic effects are **weak** and arise from paired electrons.

Measurement:

- Paramagnetism is easily measured in the lab and expressed as **magnetic moment (μ)** in **Bohr Magnetons (B.M.)**.
- The value of μ helps determine the number of unpaired electrons in the complex.
- n= Number of Unpaired Electrons

$$\mu = \sqrt{n(n+2)}$$

The significance of magnetic moment lies in:

- Providing crucial information about:
- The number of unpaired electrons in the central metal atom/ion.
- The occupied orbitals of the metal.
- Revealing the structure and geometry of complexes in certain cases.

Diamagnetic complexes:

Magnetic moment (**μ = 0**) → No unpaired electrons (all e^- paired).

Paramagnetic complexes:

Magnetic moment (**μ > 0**) → Value depends on the number of unpaired electrons (**n**).

B.M. 1.73 = μ فإن , n = 1	→ $\mu = \sqrt{1(1+2)} = 1.73$ B.M
B.M. 2.83 = μ فإن , n = 2	→ $\mu = \sqrt{2(2+2)} = 2.83$ B.M
B.M. 3.87 = μ فإن , n = 3	→ $\mu = \sqrt{3(3+2)} = 3.87$ B.M