INDEX

|  |  |  |
| --- | --- | --- |
| Sr.no | Topic | Pg.no |
| 1 | Introduction to coordination compounds | 1 |
| 2 | Werner’s theory of coordination compounds | 2 |
| 3 | Central atom | 4 |
| 4 | Lewis acids | 5 |
| 5 | Ligands | 6 |
| 6 | Coordination sphere | 7 |
| 7 | Coordination polyhedron | 8 |
| 8 | Oxidation number of central atom | 9 |
| 9 | Isomerism | 10 |
| 10 | Valence bond theory | 11 |
| 11 | Crystal field theory | 14 |
| 12 | Colour in coordination compounds | 16 |
| 13 | Bonding in metal carbonils | 19 |
| 14 | Summery | 20 |

1. Introduction to coordination compounds

In the intricate tapestry of contemporary scientific exploration, coordination compounds emerge as pivotal keystones, binding together diverse fields with their profound implications and versatile applications. This introduction sets the stage for a research-based exploration into the nuanced realms of coordination chemistry, where the interplay of metal ions and ligands orchestrates molecular symphonies that resonate across disciplines.

At its core, coordination chemistry unfolds a rich narrative of chemical bonding, reactivity, and structural intricacies. As researchers, our pursuit delves into the rational design and synthesis of these compounds, aiming not only to unveil their underlying principles but also to harness their potential for ground breaking advancements.

The significance of coordination compounds is underscored by their prevalence in nature, from essential biological processes to the geological formations that shape our world. Our paper endeavours to unravel the molecular intricacies behind these phenomena, shedding light on the role of coordination compounds in catalysis, sensing, and medicinal applications.

As we embark on this research-based journey, we navigate through recent developments, innovative methodologies, and emerging trends in coordination chemistry. The paper will serve as a compass, guiding fellow researchers through the uncharted territories of ligand design, metal-ligand cooperation, and the dynamic behaviour of these compounds under varying conditions.

By weaving together experimental findings and theoretical insights, our exploration seeks not only to deepen our understanding of coordination compounds but also to inspire novel avenues for scientific inquiry. As we celebrate the inaugural year of this research endeavour, let us collectively delve into the profound complexities and limitless possibilities encapsulated within the realm of coordination compounds

2. Werner’s theory of coordination Compounds

Central Metal Atom or Ion (Coordination Centre):

Werner introduced the concept of a central metal atom or ion (coordination centre) that acts as the core of the coordination compound. This metal centre has the ability to form chemical bonds with surrounding molecules or ions, called ligands.

Coordination Number:

Werner proposed that each central metal ion has a characteristic coordination number, which represents the maximum number of ligands that can be attached to the metal ion. The coordination number is determined by the metal ion's valence and electron configuration.

Example: [Co(F6)]-3 coordination number 6

[Co(NH3)6]+3 coordination number 6

[Fe(CO)5] coordination number 5

Primary Valence and Secondary Valence:

Werner distinguished between two types of valances associated with the central metal ion:

*Primary Valence (P):* The number of simple ions (positive or negative) associated with the central metal ion. These ions counterbalance the charge of the metal.

*Secondary Valence (S):* The number of ligands coordinated to the central metal ion.

Types of Coordination Complexes:

Werner's theory recognized two fundamental types of coordination complexes:

*Non-Ionic Coordination Complexes:* These complexes are formed by the direct union of neutral molecules (ligands) with the central metal ion.

*Ionic Coordination Complexes:* In these complexes, the ligands are charged ions (e.g., Cl-, NH₃⁺), and they bond to the central metal ion through electrostatic attraction.

Isomerism:

Werner's theory helped explain the phenomenon of isomerism in coordination compounds. He identified two main types of isomerism:

*Structural Isomerism:* Isomers with the same molecular formula but different arrangements of ligands around the central metal ion.

*Stereoisomerism:* Isomers with the same connectivity of ligands but different spatial arrangements due to the presence of chiral ligands or geometric isomerism.

*Coordination Sphere and Coordination Polyhedron:*

Werner introduced the concept of a coordination sphere, which includes the central metal ion and its coordinated ligands. The coordination polyhedron describes the geometric arrangement of the ligands around the central metal ion. Different coordination numbers give rise to different polyhedral (e.g., octahedral, tetrahedral, square planar).

*Valence Isomerism:*

Werner's theory also addressed the phenomenon of valence isomerism, where the central metal ion changes its oxidation state while keeping the same coordination number.

Coordinationentity

The central metal ion or atom is typically a transition metal or sometimes a main group element. It serves as the core of the coordination entity, providing one or more vacant orbitals (usually d or f orbitals) for bonding with the ligands. The identity of the central metal ion or atom plays a crucial role in determining the properties and reactivity of the coordination complex.

3. Central atom

*Central Atom:*

In chemistry, a central atom refers to an atom, typically in a molecule or a complex ion, that is bonded to other atoms or ions. It is the atom at the centre of a chemical species, and it forms covalent or coordinate covalent bonds with surrounding atoms or ions. The central atom is usually the least electronegative element in a molecule or complex and is often found in the centre of a Lewis structure.

*Central Ion (Coordination Centre):*

In coordination compounds or complexes, a central ion, also known as a coordination centre or central metal ion, is an ion (usually a metal cation) that forms coordinate covalent bonds with surrounding molecules or ions called ligands.

The central ion or atom plays a crucial role in coordination chemistry, where it can have varying coordination numbers and geometries depending on the nature of the ligands and the central ion itself.

4. Lewis acids

**Electron Pair Acceptance:** Lewis acids are defined by their willingness to accept a pair of electrons from another species. This electron pair can come from a molecule, an ion, or another atom.

**Incomplete Octet**: Many Lewis acids are characterized by having an incomplete valence electron shell. This means they have empty orbitals available to accept the incoming electron pair.

**Positive Charge**: Lewis acids can be positively charged ions, neutral molecules, or even negatively charged ions, depending on their electron deficiency or electron demand.

5. Ligands

**Electron-Pair Donors**: Ligands act as electron-pair donors, contributing a pair of electrons to the central metal ion or atom

**Varied Nature**: Ligands can be diverse in their chemical nature, including neutral molecules, anions, or even cations. Common examples of ligands include water (H₂O), ammonia (NH₃), chloride ions (Cl⁻), and cyanide ions (CN⁻).

**Coordination Number**: The number of ligands that can surround a central metal ion is determined by the metal's coordination number. For example, a metal with a coordination number of 6 can bond to six ligands.

**Charge**: Ligands can be neutral or charged. Charged ligands are also known as complex ions or ligand ions. Ligands with a negative charge are called anions, while those with a positive charge are called cations.

**Roles of Ligands**:

**Coordination**: Ligands coordinate with the central metal ion or atom, forming a coordination sphere that encapsulates the metal. This coordination results in the formation of a coordination complex.

**Determination of Geometry**: The choice of ligands and their arrangement around the central metal ion influence the geometry of the coordination complex. Different ligands can lead to various complex shapes, such as octahedral, tetrahedral, square planar, and more.

**Stabilization**: Ligands help stabilize the central metal ion or atom by donating electron pairs, which reduces the positive charge on the metal and increases the overall stability of the complex.

**Tuning Reactivity**: The nature of ligands can significantly affect the reactivity of the coordination complex. Different ligands can lead to variations in the chemical reactivity and catalytic properties of the complex.

**Colour and Magnetism**: Ligands can influence the colour and magnetic properties of coordination complexes. Certain ligands can cause the complex to exhibit unique colours and magnetic behaviour.

**Chirality**: Some ligands can introduce chirality into coordination complexes, making them optically active. This property is essential in fields such as asymmetric synthesis and bioinorganic chemistry.

**Binding Specificity**: In biological systems, ligands play a critical role in binding to metal ions in metalloenzymes and metalloproteinase, influencing their functions.

6. Coordination sphere

Central Metal Ion or Atom (Coordination Central): At the heart of the coordination sphere is a central metal ion or atom, which serves as the focal point of the complex. The properties of the central metal ion or atom, including its identity, charge, and coordination number, influence the overall behaviour of the coordination complex.

**Ligands:** The ligands are molecules, ions, or atoms that form coordinate covalent bonds with the central metal ion or atom. These ligands surround the central metal, and their arrangement, nature, and number determine the geometry of the coordination complex. Ligands can be neutral molecules or charged ions.

**Composition:** The coordination sphere provides information about the composition of the coordination complex, specifying which ligands are bonded to the central metal ion or atom. The type and number of ligands in the coordination sphere are crucial in defining the complex's properties.

**Charge:** The coordination sphere carries an overall charge that reflects the charge of the central metal ion or atom and the ligands. This charge helps balance the charge of the entire complex, ensuring that it is electrically neutral.

**Square Brackets**: The coordination sphere is often enclosed in square brackets, indicating that it is a distinct unit within the coordination complex. The central metal ion or atom and the ligands inside the brackets are collectively referred to as the coordination sphere.

**Coordination Number and Geometry:** The coordination number, which represents the total number of coordinate bonds formed between the central metal and the ligands, is related to the geometry of the coordination complex. Different coordination numbers correspond to different geometric arrangements, such as octahedral, tetrahedral, square planar, and others.

7. Coordination polyhedron

Central Metal Ion or Atom (Coordination Central): At the central of the coordination polyhedron is the central metal ion or atom. This metal ion or atom is the focal point of the coordination complex and serves as the core to which ligands are attached.

**Ligands:** Ligands are molecules, ions, or atoms that form coordinate covalent bonds with the central metal ion or atom. They surround the central metal and occupy specific positions in space relative to the central ion.

**Vertices**: The vertices of the coordination polyhedron represent the positions occupied by the ligands in the complex. Each vertex corresponds to a ligand, and the ligands are located at these points in three-dimensional space.

**Edges and Faces**: In a coordination polyhedron, edges connect the vertices, and faces are formed by connecting three or more vertices. These edges and faces define the boundaries of the polyhedron and help determine its shape.

**Coordination Number**: The coordination number, which is the total number of coordinate bonds formed between the central metal and the ligands, corresponds to the number of vertices in the coordination polyhedron.

**Geometry**: The coordination polyhedron reflects the geometry of the coordination complex. Different coordination numbers lead to different coordination polyhedral, each with a specific geometric shape. Common coordination geometries include octahedral, tetrahedral, square planar, and more.

**Chirality**: The coordination polyhedron can also provide information about the chirality (optical activity) of the coordination complex. Some polyhedra have mirror-image forms (enantiomers), making the complex optically active.

8. Oxidation number of central atom

**Neutral Complexes**: In many coordination complexes, the sum of the oxidation numbers of all the atoms (including the central metal atom) must equal the overall charge of the complex, which is usually zero for neutral complexes. For example, in the complex [Cu(NH₃)₄]²⁺, the sum of the oxidation numbers of copper (Cu) and nitrogen (N) must add up to +2 to match the charge of the complex.

**Charged Complexes**: For charged coordination complexes, the sum of the oxidation numbers must equal the overall charge of the complex. For example, in the complex [Fe(CN)₆]³⁻, the sum of the oxidation numbers of iron (Fe) and carbon (C) must add up to -3 to match the charge of the complex.

**Oxidation Number Rules**: To determine the oxidation number of the central metal atom, you can use a set of rules:

* The oxidation number of an un combined element is zero (e.g., O₂, N₂).
* In monatomic ions, the oxidation number is equal to the charge of the ion (e.g., Na⁺ has an oxidation number of +1).
* Hydrogen is typically assigned an oxidation number of +1.
* Oxygen is usually assigned an oxidation number of -2.
* The sum of the oxidation numbers of all atoms in a neutral molecule or complex is zero.
* The sum of the oxidation numbers of all atoms in a polyatomic ion is equal to the charge of the ion.

**Exceptions**: There are exceptions to these rules, especially in coordination complexes where the ligands can influence the oxidation state of the central metal. Some ligands are strong electron donors and can lead to a lower oxidation state of the central metal, while others are weaker donors or even electron acceptors.

**Coordination Number and Oxidation State**: The coordination number (the number of ligands bonded to the central metal) can also influence the oxidation state. For example, a central metal ion with a higher coordination number may have a lower oxidation state because it has more electron-donating ligands around it.

**Oxidation State Changes**: In redox reactions involving coordination complexes, the oxidation state of the central metal atom can change as it gains or loses electrons. These changes are important in understanding the reactivity of coordination compounds.

9. Isomerism

**Structural Isomerism:**

Structural isomerism arises when coordination complexes with the same chemical formula have different connectivity of atoms and/or different arrangements of ligands around the central metal ion. There are several subtypes of structural isomerism:

**Coordination Sphere Isomerism**: In this type of isomerism, the connectivity of ligands within the coordination sphere changes. For example, in [Co(NH₃)₆]³⁺ and [Co(en)₃]³⁺, where en = ethylenediamine, the ligands are different, resulting in coordination sphere isomerism.

**Linkage Isomerism**: This occurs when a ligand can bind to the central metal ion through different donor atoms. For instance, in [Pt(NH₃)₄Cl₂] and [Pt(NH₃)₄Cl(NO₂)], the nitrate (NO₂) ligand can coordinate through either nitrogen or oxygen atoms, leading to linkage isomerism.

**Ionization Isomerism**: Ionization isomerism occurs when a complex can undergo an equilibrium reaction with an isomeric complex in which a ligand inside the coordination sphere is replaced by an anionic or cationic species. For example, [Co(NH₃)₄(H₂O)Cl]²⁺ and [Co(NH₃)₄Cl₂]⁺ are ionization isomers because they can interconvert by the exchange of a chloride ion and a water molecule.

**Stereoisomerism:** Stereoisomerism involves compounds with the same connectivity of atoms but different spatial arrangements or orientations of the ligands around the central metal ion. Stereoisomerism can be further divided into two subtypes:

**Geometric Isomerism (Cis-Trans Isomerism**): Geometric isomers have the same connectivity of ligands but differ in the spatial arrangement of those ligands around the central metal. This type of isomerism often occurs in coordination complexes with coordination numbers of 4 or 6. Common examples include cis and Trans isomers.

**Optical Isomerism (Enantiomerism**): Optical isomerism arises when a coordination complex lacks a plane of symmetry, resulting in non-superimposable mirror-image structures known as enantiomers. Enantiomers have identical connectivity of atoms but differ in their three-dimensional spatial arrangement. They rotate plane-polarized light in opposite directions and have different chiral properties.

10. Valence bond theory

**Atomic Orbitals:**

Valence Bond Theory is built upon the concept of atomic orbitals, which are regions of space around an atomic nucleus where there is a high probability of finding electrons. The main atomic orbitals involved in VB theory are s (spherical), p (dumbbell-shaped), and, to some extent, d (complex shapes).

**Hybridization:**

In VB theory, atomic orbitals can combine or hybridize to form new hybrid orbitals with different shapes and orientations.Hybridization is a process that results in hybrid orbitals that can better explain the geometry and bonding in molecules.Formation of Covalent Bonds in Valence Bond Theory:

**Covalent Bond Formation:**

According to VB theory, a covalent bond is formed when two atoms approach each other closely enough for their valence atomic orbitals to overlap. The electrons in these overlapping orbitals are shared between the two atoms, creating a bond.

**Overlap of Atomic Orbitals:**

The strength and stability of a covalent bond are determined by the extent of overlap between the atomic orbitals of the bonding atoms. Sigma (σ) bonds are formed when orbitals overlap head-on along the bond axis, while pi (π) bonds result from side-to-side overlap of parallel p orbitals.

**Hybrid Orbitals:**

VB theory introduces the concept of hybridization, where atomic orbitals from the same atom (usually s, p, and/or d orbitals) combine to form hybrid orbitals. These hybrid orbitals have different shapes and are used to explain the geometry of molecules. Common hybridization states include sp, sp², and sp³. Geometry and Molecular Shape:

**VSEPR Theory**:

Valence Bond Theory can be combined with the VSEPR (Valence Shell Electron Pair Repulsion) theory to determine the molecular geometry of compounds. VSEPR theory considers both bonding and non-bonding electron pairs around the central atom to predict molecular shapes.

**Strengths**:

Valence Bond Theory provides a qualitative and intuitive understanding of covalent bonding.

It can explain phenomena like the formation of sigma and pi bonds and the concept of resonance in molecules.

**Magnetic properties**

**Paramagnetism:**

Paramagnetic coordination compounds contain one or more unpaired electrons in their molecular orbitals. Unpaired electrons have intrinsic magnetic moments associated with their spin. In the presence of an external magnetic field, these magnetic moments align with the field, causing the compound to be attracted to the magnet. The degree of paramagnetism is directly proportional to the number of unpaired electrons and their magnetic moments. Examples of paramagnetic coordination compounds include [Fe(H₂O)₆]³⁺ and [Cu(NH₃)₄]²⁺.

**Diamagnetism:**

Diamagnetic coordination compounds contain no unpaired electrons in their molecular orbitals. Diamagnetic compounds are weakly repelled by an external magnetic field. This repulsion arises from the slight induction of opposing magnetic moments in response to the external field. Diamagnetic behaviour is a common characteristic of coordination compounds, as most transition metal complexes involve electron pairing in their molecular orbitals. Examples of diamagnetic coordination compounds include [Ni(CO)₄] and [Cu(en)₃]²⁺, where en is ethylenediamine. Ferromagnetism and Anti ferromagnetism (Rare):

Coordination compounds that exhibit ferromagnetism or anti ferromagnetism are relatively rare and typically involve metals with unpaired d electrons. Ferromagnetic compounds have unpaired electrons with parallel spins, leading to alignment of magnetic moments in the same direction, resulting in a net magnetic moment. These compounds are attracted to a magnetic field.

Antiferromagnetic compounds have unpaired electrons with antiparallel spins, leading to the cancellation of magnetic moments, resulting in no net magnetic moment. These compounds are not attracted to a magnetic field.

Examples of ferromagnetic coordination compounds are scarce but include some transition metal complexes with strong exchange interactions.

Antiferromagnetic coordination compounds are also rare and involve complex arrangements of spins that result in the cancellation of net magnetic moments.

**Limitations of valence bond theory**

**Limited Quantitative Predictive Power:** Valence Bond Theory provides a qualitative understanding of chemical bonding and structure, but it lacks the quantitative predictive power of Molecular Orbital Theory (MO theory). MO theory can accurately calculate bond energies and electronic properties.

**Limited Scope for Transition Metal Complexes:** VB theory struggles to explain the bonding in transition metal complexes with highly delocalized and complex electronic structures. These complexes often involve strong interactions between metal d orbitals and ligand orbitals, which are better described by MO theory.

**Inadequate Treatment of Excited States:** VB theory primarily focuses on the ground state of molecules and does not provide a robust framework for describing excited states, such as those involved in photochemistry and spectroscopy. MO theory is better suited for this purpose.

**Difficulty in Describing Complex Resonance**: In cases of resonance where multiple Lewis structures contribute significantly to the electronic structure of a molecule or ion, VB theory becomes cumbersome and does not provide a concise description.

**Does Not Address Molecular Properties**: While VB theory can explain how bonds form and the shapes of molecules, it does not directly address molecular properties such as magnetic behaviour, molecular orbital diagrams, or the interaction of molecules with electromagnetic radiation (spectroscopy). MO theory is more adept at describing these properties.

**Hybridization as an Ad Hoc Concept**: The concept of hybridization, which is integral to VB theory, is sometimes considered ad hoc. Hybridization assumes that atomic orbitals mix to form hybrid orbitals, and the process is somewhat arbitrary, leading to concerns about its physical significance.

**Neglects Electron Correlation Effects:** VB theory treats electrons as being localized in specific bonds or between atoms, neglecting electron correlation effects. MO theory, on the other hand, considers the behaviour of all electrons in the molecular system.

**Difficulties with Molecular Geometry**: While VB theory can provide qualitative explanations for molecular geometries, it may not predict bond angles and bond lengths as accurately as MO theory.

**Complexity of Polyatomic Molecules**: VB theory becomes increasingly complex and less useful for polyatomic molecules with many atoms and multiple bonding interactions. Despite these limitations, Valence Bond Theory remains a valuable and pedagogically important tool for teaching and understanding chemical bonding, especially in simple covalent compounds. In many cases, it can provide qualitative insights into molecular structure and bonding. However, for more complex systems and accurate quantitative predictions, Molecular Orbital Theory is often preferred.

11. Crystal field theory

Central Metal Ion: In CFT, the central metal ion is the focal point of the coordination complex. It typically has partially filled d orbitals, which are involved in bonding with ligands.

**Ligands**: Ligands are molecules or ions that coordinate to the central metal ion through the donation of electron pairs to form coordinate bonds. Ligands can be classified as strong-field or weak-field ligands based on their ability to cause splitting of the metal's d orbitals.

**Crystal Field Splitting**: One of the central concepts of CFT is crystal field splitting, which refers to the energy difference between the five d orbitals of the central metal ion in a spherical or octahedral field of ligands. This splitting results from electrostatic interactions between the negatively charged electrons in the ligands and the positively charged metal ion.

**Octahedral Field**: In octahedral coordination complexes, such as [Co(NH₃)₆]³⁺, the d orbitals are split into two energy sets: three lower-energy orbitals (t2g set) and two higher-energy orbitals (eg set). The energy difference between the two sets is known as Δ₀ (delta naught). Ligands that cause large crystal field splitting are called strong-field ligands, and they typically lead to low-spin complexes, where electrons preferentially occupy the lower-energy t2g orbitals before the higher-energy eg orbitals. Ligands that cause small crystal field splitting are called weak-field ligands and often lead to high-spin complexes, where electrons occupy both t2g and eg orbitals.

Tetrahedral Field: In tetrahedral coordination complexes, such as [NiCl₄]²⁻, the d orbitals are also split into two sets: two lower-energy orbitals and three higher-energy orbitals. However, the energy difference between these sets is smaller than in octahedral complexes. Tetrahedral complexes typically have higher-spin configurations due to the smaller energy gap between the sets of d orbitals.

Consequences and Applications:

**Colour:** CFT explains the colour of transition metal complexes by linking electronic transitions between the split d orbitals to specific absorption wavelengths. Complexes with unpaired electrons in the eg set tend to absorb visible light and appear colored.

**Magnetic Behavior:** CFT helps explain the magnetic behaviour of coordination complexes. Low-spin complexes have fewer unpaired electrons and are diamagnetic (weakly repelled by a magnetic field), while high-spin complexes are paramagnetic (attracted to a magnetic field) due to their greater number of unpaired electrons.

**Stability:** The relative stability of different coordination complexes can be predicted using CFT. Complexes with lower crystal field splitting energy (Δ₀) are often more stable.

Electronic Configurations: CFT assists in determining the electronic configurations of transition metal complexes based on the number of electrons and the crystal field splitting.0

12. Colour in coordination compounds

Copper ions (Cu²⁺) often produce blue or green colors in coordination compounds. For example:

[Cu(H₂O)₆]²⁺ is blue.

[Cu(NH₃)₄]²⁺ is deep blue.

[CuCl₄]²⁻ is yellow-green.

Chromium Compounds:

Chromium ions (Cr³⁺) are known for producing various colors depending on their oxidation state and ligands. For example:

[Cr(H₂O)₆]³⁺ is violet.

[Cr(en)₃]³⁺ (en = ethylenediamine) is dark green.

[CrO₄]²⁻ is yellow.

Nickel Compounds:

Nickel ions (Ni²⁺) can produce green or blue colors in coordination compounds. For example:

[Ni(H₂O)₆]²⁺ is green.

[Ni(en)₃]²⁺ is green.

Cobalt Compounds:

Cobalt ions (Co²⁺ and Co³⁺) are known for their pink, blue, or green colors. For example:

[Co(H₂O)₆]²⁺ is pink.

[Co(NH₃)₆]³⁺ is yellow.

[CoCl₆]³⁻ is blue.

Iron Compounds:

Iron ions (Fe²⁺ and Fe³⁺) can produce various colors, including orange, brown, and green. For example:

[Fe(H₂O)₆]²⁺ is pale green.

[Fe(CN)₆]³⁻ is deep brown.

[FeCl₄]²⁻ is yellow.

Manganese Compounds:

Manganese ions (Mn²⁺ and Mn³⁺) can produce pink, purple, or brown colors. For example:

[Mn(H₂O)₆]²⁺ is pale pink.

[MnO₄]⁻ is dark purple.

[Mn²⁺(aq)] is pale pink.

Vanadium Compounds:

Vanadium ions (V²⁺ and V³⁺) can produce various colors, including green, blue, and yellow. For example:

[V(H₂O)₆]²⁺ is blue.

[VCl₆]³⁻ is green.

[VO₂⁺(aq)] is yellow.

The specific colour of a coordination compound depends on factors such as the central metal ion, its oxidation state, the type of ligands, and the geometry of the complex. The interaction between the d orbitals of the metal and the ligands causes electronic transitions that absorb certain wavelengths of light and give rise to the observed colour.

*Limitations of crystal field theory*

**Neglect of Covalency**: CFT assumes that the interaction between the central metal ion and ligands is purely ionic, with no sharing of electrons between the metal and ligands. In reality, many coordination compounds exhibit covalent bonding, where electrons are shared between the metal and ligands. CFT does not account for these covalent interactions, which are better described by Molecular Orbital Theory (MO theory).

**Weak-Field vs. Strong-Field Ligands**: CFT classifies ligands as either weak-field or strong-field based solely on their ability to cause crystal field splitting. This classification is somewhat arbitrary and does not consider the full range of ligand properties or the covalent nature of metal-ligand bonding.

**Inability to Predict Magnetic Behaviour**: While CFT can qualitatively explain the magnetic properties of coordination compounds, it cannot predict the magnetic behavior of all complexes accurately. It cannot account for cases where other factors, such as exchange interactions, dominate the magnetic behaviour.

**Limitations in Predicting Electronic Configurations**: CFT does not provide a detailed description of the electronic configurations of transition metal complexes, especially those with significant covalent character. MO theory is more suitable for predicting electronic configurations accurately.

**Does Not Address Molecular Geometry**: CFT focuses primarily on the splitting of d orbitals and does not provide insights into the molecular geometry of coordination complexes. Molecular Orbital Theory and Ligand Field Theory are better suited for predicting and explaining molecular geometries.

**Complexity of Transition Metal Complexes:** CFT becomes less accurate and less useful when applied to highly complex transition metal complexes involving multiple metal centres or ligands with intricate structures. MO theory can handle such complexity more effectively.

**Ignores Electron-Electron Repulsions:** CFT neglects electron-electron repulsions within the d orbitals, which can play a significant role in determining the actual electronic structure of coordination compounds, especially when many d electrons are involved.

**Limited Application to Non-Transition Metal Complexes**: CFT is primarily designed for transition metal complexes. It is less applicable to non-transition metal complexes or compounds involving main group elements.

**Limited Treatment of Excited States**: CFT primarily focuses on the ground state electronic configuration and does not provide a systematic approach to describing excited states or electronic transitions, which are important in spectroscopy and photochemistry. **Cannot Explain Complex Spectroscopic Data**: For complex coordination compounds, CFT often falls short in explaining complex spectroscopic data and phenomena, such as ligand-to-metal charge transfer transitions.

13. Bonding in metal carbonils

**Coordination Bonds**: In metal carbonyls, the central metal atom or ion forms coordinate covalent bonds with one or more carbonyl ligands. A coordinate covalent bond is formed when the metal atom donates a pair of electrons to a vacant anti bonding orbital on the carbon monoxide ligand.

**Presence of Carbonyl Ligands**: Carbonyl ligands (CO) consist of a carbon atom bonded to an oxygen atom through a triple bond (C≡O). The oxygen atom bears a partial negative charge, while the carbon atom carries a partial positive charge. The carbon atom's lone pair is available for coordination with the metal.

**Back bonding:** One of the essential features of metal carbonyls is back bonding or π-donation, where the metal d orbitals (particularly the empty dπ orbitals) interact with the π anti bonding orbitals of the carbonyl ligands. This interaction reinforces the metal-carbon bond and helps stabilize the complex.

**Types of Bonds in Metal Carbonyls:**

**σ-Bonding**: Metal-carbon σ-bonds are formed by the overlap of a metal's atomic orbitals (usually d orbitals) with the σ-bonding orbitals of the carbonyl ligands. These σ-bonds are the primary bonding interactions in metal carbonyls.

**π-Bonding**: Metal-carbon π-bonds result from the interaction between the metal's dπ orbitals and the π anti bonding orbitals of the CO ligands. This π-back bonding contributes to the stability of the complex.

**Bond Strength and Stability:**

The strength and stability of metal carbonyl complexes depend on factors such as the nature of the metal, the number of carbonyl ligands, and the availability of d orbitals on the metal for back bonding. Generally, metals with partially filled d orbitals are more likely to form stable carbonyl complexes.

**Applications**:

**Catalysis**: Metal carbonyls are important catalysts in various industrial processes, including hydro formulation and carbonization reactions.

**Synthetic Chemistry**: They are used as reagents in organic synthesis, such as in the synthesis of acyl derivatives and as sources of pure carbon monoxide.

**Electronics**: Some metal carbonyls are used in the electronics industry for the deposition of metal films in microelectronics and semiconductors.

14. Summery

Coordination compounds consist of a central metal atom or ion bonded to surrounding molecules or ions called ligands. These ligands donate electron pairs to form coordinate covalent bonds with the central metal, stabilizing the complex.

Formation of Coordinate Bonds: The primary bonding mechanism in coordination compounds is the formation of coordinate covalent bonds between the metal and the ligands. These bonds result from the donation of electron pairs from ligands to vacant orbitals on the metal.

The coordination number refers to the total number of coordinate bonds formed between the central metal and its surrounding ligands. It determines the geometry and properties of the complex.

Ligands can be neutral molecules, anions. They vary in their electron-donating abilities and can influence the stability and reactivity of the coordination complex.

Chelating ligands are special ligands that can form multiple coordinate bonds with a single metal centre. This property enhances the stability of the complex and is commonly observed in biological systems.

The spatial arrangement of ligands around the central metal is defined by the coordination geometry. Common geometries include octahedral, tetrahedral, square planar, and others.

Coordination compounds exhibit various types of isomerism, including structural isomerism and stereoisomerism, which arise from different arrangements of ligands around the central metal.

Many coordination compounds are coloured due to electronic transitions within the d orbitals of the central metal. Their magnetic behaviour, whether paramagnetic or diamagnetic, can be explained by the presence of unpaired electrons.

Crystal Field Theory is a model used to describe the electronic structure and magnetic properties of coordination compounds. It focuses on the splitting of d orbitals in the presence of ligands and helps explain colour and magnetism.

Coordination compounds have a wide range of applications, including catalysis, industrial processes, materials science, bioinorganic chemistry, and medicine (e.g., chemotherapy drugs).