

How Many Unpaired Electrons Are In The High-spin State Of W^{2+} In An Octahedral Field? Unpaired Electrons

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Understanding the electronic configuration of transition metal ions in various crystal fields is fundamental in inorganic chemistry, especially when analyzing magnetic properties, spectroscopic behaviors, and chemical reactivity. One particularly interesting case involves the tungsten(II) ion, W^{2+} , situated within an octahedral crystal field. Determining how many unpaired electrons W^{2+} possesses in its high-spin state provides insight into its magnetic moment and overall electronic structure. This article explores the electronic configuration of W^{2+} in an octahedral environment, the concept of high-spin versus low-spin states, and the factors influencing the number of unpaired electrons.

Fundamentals of Transition Metal Electronic Configurations

Transition metals are characterized by their partially filled d-orbitals, which play a crucial role in their chemical and physical properties. The electronic configuration of a transition metal ion depends on its oxidation state and the ligand field environment.

- Atomic number of tungsten (W): 74
- Ground state electron configuration of W: $[Xe] 4f^{14} 5d^4 6s^2$

When tungsten forms ions, electrons are removed primarily from 6s and 5d orbitals, affecting the number of unpaired electrons and magnetic properties.

Oxidation State and Electron Count for W^{2+}

In the W^{2+} ion:

- Oxidation state: +2
- Electron removal: Two electrons are removed from the neutral atom's configuration.

Starting with the neutral tungsten atom:

- [Xe] 4f¹⁴ 5d⁴ 6s²

Removing two electrons typically involves:

1. First, removing electrons from the 6s orbital.
2. If necessary, removing from the 5d orbital.

In transition metals, the common removal sequence is 6s electrons first, followed by 4f or 5d electrons.

For W²⁺:

- Remove two electrons from 6s²: resulting in [Xe] 4f¹⁴ 5d⁴

Therefore, the electronic configuration of W²⁺ in its ground state is:

- [Xe] 4f¹⁴ 5d⁴

The 4f shell is filled, and the remaining electrons occupy the 5d orbitals.

Crystal Field Theory and Octahedral Ligand Environment

When W²⁺ is situated in an octahedral ligand field, the five degenerate d-orbitals split into two energy levels:

- t_{2g} orbitals: lower energy (d_{xy}, d_{xz}, d_{yz})
- e_g orbitals: higher energy (d_{x²-y²}, d_{z²})

The magnitude of this splitting (Δ_0) influences whether electrons pair up in lower energy orbitals (low-spin) or occupy higher energy orbitals to maximize unpaired electrons (high-spin).

High-Spin vs. Low-Spin Configurations

- High-Spin State: Electrons occupy all available orbitals to maximize unpaired electrons, occurring when ligand field splitting is small.
- Low-Spin State: Electrons pair in lower energy orbitals, favored when ligand field splitting is large.

The nature of ligands and the metal's electronic configuration determine whether the complex adopts a high-spin or low-spin state.

Electronic Configuration of W^{2+} in an Octahedral Field

Given W^{2+} 's configuration: $[Xe] 4f^{14} 5d^4$

- The 4f electrons are core electrons and generally do not participate significantly in bonding or ligand field splitting.
- The valence electrons involved in bonding are primarily the 5d electrons.

Thus, the relevant configuration for magnetic and ligand field considerations is:

- $5d^4$

The key question is whether these 5d electrons prefer to be high-spin or low-spin in an octahedral environment.

Determining the Number of Unpaired Electrons in W^{2+}

Step 1: Electron configuration of $5d^4$

In a free ion, $5d^4$ electrons can be arranged to maximize or minimize pairing:

- High-spin configuration: Electrons occupy separate orbitals with parallel spins to maximize unpaired electrons.
- Low-spin configuration: Electrons pair up in lower energy orbitals.

Step 2: Ligand field considerations

- For $5d^4$ in an octahedral field, the energy gap Δ_o and pairing energy (P) determine the spin state.
- 5d orbitals are more diffuse and experience stronger ligand interactions than 3d orbitals, often favoring low-spin configurations with strong field ligands.
- However, in the case of weak field ligands (like halides), high-spin states are favored.

Step 3: High-spin state of W^{2+}

In the high-spin state, electrons occupy all five d orbitals with maximum unpaired electrons:

- Electron distribution: $t_{2g}^3 e_g^1$ (if considering the splitting), but for 4 electrons, the Hund's rule favors maximizing unpaired electrons.

Assuming the high-spin state:

- Each of the four electrons occupies separate orbitals with parallel spins, resulting in:

Number of unpaired electrons = 4

Step 4: Magnetic properties

- The magnetic moment (μ) can be estimated using the spin-only formula:

$$\mu_{\text{spin-only}} = \sqrt{n(n+2)} \text{ Bohr Magnetons}$$

where n is the number of unpaired electrons.

- For 4 unpaired electrons:

$$\mu_{\text{spin-only}} = \sqrt{4(4+2)} = \sqrt{24} \approx 4.90 \mu_B$$

This value indicates a high-spin configuration.

Conclusion: Number of Unpaired Electrons in W^{2+} High-Spin State

Based on the above analysis:

- The W^{2+} ion in an octahedral high-spin environment has 4 unpaired electrons.

This configuration significantly influences its magnetic properties, spectroscopic features, and chemical reactivity.

Additional Factors Influencing Electron Spin State

Several factors can sway the electron arrangement in W^{2+} complexes:

- **Ligand Field Strength:** Strong field ligands (like CN^-) tend to produce low-spin states, reducing unpaired electrons.
- **Geometry and Coordination Number:** Deviations from perfect octahedral symmetry can alter splitting and electron distribution.
- **Electron Correlation Effects:** Fine electronic interactions can influence the spin state.

Implications of Unpaired Electrons in W^{2+} Complexes

The number of unpaired electrons affects various properties:

- Magnetic Behavior: W^{2+} complexes with 4 unpaired electrons are paramagnetic.
- Spectroscopic Features: Electronic transitions depend on the spin state and electron configuration.
- Reactivity: Magnetic properties can influence catalytic activity and bonding tendencies.

Summary Table: W^{2+} in an Octahedral High-Spin State

Property	Description
Electron configuration	[Xe] 4f ¹⁴ 5d ⁴
Relevant electrons	5d electrons (4 electrons)
Spin state	High-spin
Number of unpaired electrons	4
Magnetic moment (approximate)	4.90 μ_B

Final Remarks

Understanding the number of unpaired electrons in transition metal complexes like W^{2+} in an octahedral high-spin state is essential for predicting their magnetic and electronic behaviors. The analysis reveals that W^{2+} , in a high-spin octahedral environment, possesses four unpaired electrons, contributing to its paramagnetic nature and influencing its chemical properties. This knowledge aids inorganic chemists in designing complexes with desired magnetic and spectroscopic characteristics, expanding applications in catalysis, materials science, and magnetic resonance technologies.

Keywords: W^{2+} , unpaired electrons, high-spin state, octahedral field, transition metals, electronic configuration, magnetic properties, ligand field theory, crystal field splitting, paramagnetism

Frequently Asked Questions

How many unpaired electrons does W^{2+} have in its high-spin state within an octahedral field?

W^{2+} in a high-spin state within an octahedral field has two unpaired electrons.

What is the electronic configuration of W^{2+} in an octahedral crystal field?

The electronic configuration of W^{2+} in an octahedral field is typically $(t_{2g})^4(eg)^2$, with two unpaired electrons in the t_{2g} orbitals in the high-spin state.

Why does W^{2+} exhibit unpaired electrons in an octahedral field?

W^{2+} exhibits unpaired electrons because its electron pairing energy is higher than the crystal field splitting, favoring a high-spin configuration with unpaired electrons.

How does the high-spin state influence the number of unpaired electrons in W^{2+} ?

In the high-spin state, electrons occupy higher energy orbitals to minimize pairing, resulting in more unpaired electrons—in the case of W^{2+} , typically two unpaired electrons.

What is the significance of unpaired electrons in W^{2+} in terms of magnetic properties?

The presence of unpaired electrons in W^{2+} confers paramagnetism, making the ion attracted to magnetic fields.

How does the electron configuration of W^{2+} compare with that of W^{3+} in an octahedral field?

W^{2+} has fewer unpaired electrons (two) compared to W^{3+} , which typically has three unpaired electrons in a high-spin octahedral field.

What factors determine whether W^{2+} adopts a high-spin or low-spin configuration?

The magnitude of the crystal field splitting energy relative to electron pairing energy determines the spin state; for W^{2+} , a smaller splitting favors a high-spin configuration with unpaired electrons.

Additional Resources

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Understanding the electronic configuration of transition metal ions is fundamental to predicting their magnetic properties, reactivity, and overall behavior in various chemical contexts. Among these, tungsten ions like W^{2+} present intriguing cases, especially when situated within an octahedral crystal field environment. A question that frequently arises among students and chemists alike is: How many unpaired electrons are present in the high-spin state of W^{2+} in an octahedral field? This article seeks to explore this question in depth, providing a comprehensive, yet accessible, overview rooted in crystal field theory, electron configurations, and magnetic considerations.

The Significance of Electron Spin and Unpaired Electrons

Before diving into the specifics of W^{2+} , it's essential to understand the broader context of unpaired electrons and their significance.

- **Unpaired Electrons:** Electrons occupying degenerate orbitals singly, with parallel spins, are termed unpaired. Their presence directly influences the magnetic properties of the ion – unpaired electrons contribute to paramagnetism, while paired electrons lead to diamagnetism.
- **High-Spin vs. Low-Spin Configurations:** Transition metal complexes can adopt high-spin or low-spin states depending on the ligand field strength, electron pairing energy, and the electronic configuration. High-spin states feature maximum unpaired electrons, resulting from weaker ligand fields that favor electron separation.
- **Relevance in Chemistry:** The number of unpaired electrons affects reactivity, spectroscopic properties, and magnetic behavior, making their determination vital in inorganic chemistry.

Understanding Tungsten's Electron Configuration

Tungsten (W) has an atomic number of 74. Its neutral atom configuration in the ground state is:

$[Xe] 4f^{14} 5d^4 6s^2$

In ionized states, especially in W^{2+} , electrons are removed from the outer shells, significantly affecting the electronic structure.

- W^{2+} Electron Configuration:

Removing two electrons typically involves the 6s and possibly the 5d electrons, depending on the energy considerations and the specific environment.

- Likely Electron Configuration for W^{2+} :

$[Xe] 4f^{14} 5d^2$

This is based on the general trend of electron removal from the outermost s and d orbitals.

Crystal Field Theory and Octahedral Ligand Environment

The behavior of W^{2+} in a complex is profoundly influenced by the ligand environment. When W^{2+} is situated within an octahedral ligand field, the d-orbitals split into two sets:

- t_{2g} : Lower energy set, comprising (d_{xy}) , (d_{xz}) , and (d_{yz}) orbitals.
- e_g : Higher energy set, comprising (d_{z^2}) and $(d_{x^2 - y^2})$ orbitals.

This splitting influences how electrons fill the orbitals, determining whether the complex adopts a high-spin or low-spin state.

Factors Determining High-Spin or Low-Spin States

- Ligand Field Strength: Ligands are characterized as strong or weak field based on their ability to split the d-orbitals. Weak field ligands (like halides) tend to produce high-spin complexes, while strong field ligands (like cyanide) favor low-spin configurations.

- Electron Pairing Energy (P): The energy cost of pairing electrons influences the spin state. When the ligand field splitting energy (Δ_{oct}) is less than P , high-spin states are favored; if $\Delta_{oct} > P$, low-spin states are more stable.

- Nature of W^{2+} Complexes: Tungsten typically forms complexes with ligands that produce relatively weak fields, often favoring high-spin states, particularly with halide or similar ligands.

Electron Configuration of W^{2+} in an Octahedral Field

Given the electron configuration of W^{2+} as $(5d^2)$, the placement of these electrons within the octahedral field determines the number of unpaired

electrons.

Step-by-step analysis:

1. Start with the free ion configuration: $(5d^2)$.

2. In an octahedral crystal field:

- The 5d electrons will occupy the split orbitals based on the competition between (Δ_{oct}) and pairing energy (P) .

3. High-spin scenario:

- When (Δ_{oct}) is small (weak field ligands), electrons occupy the degenerate orbitals singly before pairing, following Hund's rule.

- For $(5d^2)$, this results in:

- Each electron occupying separate orbitals with parallel spins, leading to maximum unpaired electrons.

4. Filling of orbitals:

- The two electrons occupy different t_{2g} orbitals with parallel spins.

5. Result:

- Number of unpaired electrons = 2.

Quantifying Unpaired Electrons in W^{2+} High-Spin Octahedral Complex

Based on the above reasoning:

- The high-spin state of W^{2+} in an octahedral field contains 2 unpaired electrons.

- This configuration aligns with the electron arrangement:

$[t_{2g}^2 \text{ (with both electrons unpaired)}]$

$[e_g^0 \text{ (empty)}]$

Magnetic Properties and Experimental Evidence

The number of unpaired electrons correlates with the magnetic moment:

- Magnetic moment (μ) :

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

where n is the number of unpaired electrons, and μ_B is the Bohr magneton.

- For 2 unpaired electrons:

$$\mu = \sqrt{2(2+2)} = \sqrt{8} \approx 2.83 \mu_B$$

- Experimental magnetic measurements of W^{2+} complexes support the presence of two unpaired electrons, confirming the high-spin state.

Implications and Applications

Understanding the unpaired electron count in W^{2+} complexes is not merely academic; it influences:

- Magnetic behavior: Paramagnetism in such compounds can be harnessed in magnetic materials or sensors.

- Reactivity: Unpaired electrons often participate in bonding and redox reactions.

- Spectroscopy: Electronic transitions involving unpaired electrons produce characteristic absorption spectra.

- Catalysis: Transition metal complexes with specific spin states can serve as catalysts in various industrial processes.

Summary and Final Remarks

In conclusion, the high-spin state of W^{2+} within an octahedral ligand field features two unpaired electrons. This configuration stems from the electron arrangement of the $5d^2$ configuration, influenced heavily by the ligand field strength and the associated electron pairing energies. Recognizing the number of unpaired electrons aids in predicting magnetic properties, reactivity, and spectroscopic behavior of tungsten complexes, making it a cornerstone concept in inorganic chemistry.

The intricate balance between electron configurations, ligand field effects, and physical properties exemplifies the nuanced beauty of transition metal chemistry. As research advances, such foundational knowledge continues to underpin developments in materials science, catalysis, and other technological innovations.

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