

Crystal Field Theory Chemistry Questions with Solutions

Q1. Which of the following compound is paramagnetic?

- a.) Hexa amine chromium (III) ion
- b.) Tetraamminezinc (II) ion
- c.) Tetracyanonickelate (II) ion
- d.) Diammine silver (I) ion

Correct Answer- (a.) Hexa amine chromium (III) ion.

Explanation– A complex is paramagnetic due to the presence of unpaired electrons. Chromium contains 3 unpaired electrons.

Q2. Crystal field stabilization energy for high spin d⁴ octahedral complex is:

a.) $- 1.8 \Delta_0$ b.) $- 1.6 \Delta_0 + P$ c.) $-1.2 \Delta_0$ d.) $-0.6 \Delta_0$

Correct Answer– (d.) $-0.6 \Delta_0$ Explanation–

 $\frac{1}{d \text{-orbitals in symmetrical}} \xrightarrow{1}_{d \text{$

CFSE = 3 $(-0.4)\Delta_0 + 0.6\Delta_0$ = $-1.2\Delta_0 + 0.6\Delta_0 = -0.6\Delta_0$

Q3. Which one of the following statements is FALSE?

a.) In an octahedral crystal field, the d electrons on a metal ion occupy the e_g set of orbitals before occupying the t_{2g} set of orbitals.

b.) Diamagnetic metal ions cannot have an odd number of electrons.

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c.) Low spin complexes can be paramagnetic.

d.) In high spin octahedral complexes, Δ_{oct} is less than the electron pairing energy and is relatively very small.

Correct Answer– (a.) In an octahedral crystal field, the d electrons on a metal ion occupy the e_g set of orbitals before occupying the t_{2g} set of orbitals.

Q4. What will be CFSE for the d⁶ high spin complex for both tetrahedral and octahedral complexes?

- a.) 0.6, 0.6
- b.) 0.4, 0.4
- c.) 0.4, 0.6
- d.) 0.6, 0.4

Correct Answer- (c.) 0.4, 0.6.

Q5. According to crystal field theory-

- a.) The order of increasing field strength of ligands is $F^- > H_2O > NH_3$.
- b.) If pairing energy exceeds the magnitude of crystal field splitting, then pairing occurs.
- c.) d⁴ to d⁷ coordination entities are more stable for the strong field than weak field cases.
- d.) Tetrahedral complexes have sufficiently large splitting energy to force pairing, and therefore, high spin configurations are rarely observed.

Correct Answer– (c.) d^4 to d^7 co-ordination entities are more stable for the strong field as compared to weak field cases.

Q6. Fill in the blank.

The electronic configuration of the central atom is K₄(Fe(CN)₆] on crystal field theory is ____.

Answer. The electronic configuration of the central atom is $K_4(Fe(CN)_6]$ on crystal field theory is $t_{2g}^6 e_g^0$.

Q7. State True or False.

Strong field ligands, such as CN⁻ usually produce low spin complexes and large crystal field splitting.

Answer. True.

Strong field ligands, such as CN⁻ usually produce low spin complexes and large crystal field splitting.

Q8. What are the limitations of crystal field theory?

Answer. The limitations of crystal field theory are as follows:

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- This theory is applicable to metal ions with d-orbitals and does not explain s- and p-orbitals.
- It does not explain z bonding in the coordination compounds.
- This theory considers electrostatic attraction between central metal ion and ligands, hence considering only ionic bonds between them but does not account for covalent nature between them or coordínate bonds.
- Water (H₂O) is a stronger ligand than OH, which this theory cannot explain satisfactorily.

Q9. Explain by giving a suitable example for Crystal field splitting.

Answer. The presence of ligands causes the splitting of degenerate energy levels. When a ligand approaches a transition metal ion, the degenerate d-orbitals split into two sets, one with lower energy and one with higher energy which is referred to as crystal field splitting, and the difference between the lower and higher energy sets is referred to as crystal field splitting energy (CFSE).



Example: 3d⁵ of Mn²⁺

Q10. On the basis of crystal field theory, write the electronic configuration of d⁴ in terms of t_{2g} and e_{q} in an octahedral field when $\Delta 0 < P$.

Answer. The magnitude of Δ_0 decides the actual configuration of d-orbitals with the help of mean pairing energy.

If $P < \Delta_{0,}$ then pairing of electrons occurs within the same set and forms low spin complexes due to strong-field ligands. Therefore, it becomes more energetically favourable for the fourth electron to occupy a t_{2g} orbital with configuration $t_{2g}^4 e_g^0$.

Q11. If Δ_0 is the octahedral crystal field splitting energy. Then what will be the CFSE for Fe(CN)₆]⁴?

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Answer. Fe is in +2 oxidation state, and therefore the configuration will be $3d^6$. Since the ligand is a strong field ligand, the excitation energy is greater than the pairing energy. Therefore, the configuration is $t_{2g}^6 e_g^0$. CFSE= $6 \times (-0.4\Delta_0) = -2.4 \Delta_0$.

Q12. How is the crystal field splitting energy for octahedral(Δ_0) and tetrahedral (Δ_t) complexes related?

Answer. Splitting in tetrahedral complexes is 2/3rd of the octahedral complex.

Therefore, for one ligand splitting on octahedral

For one ligand splitting in tetrahedral is

$$\Delta t = 4 \times \frac{2}{3} \left(\frac{\Delta_0}{6} \right) = \frac{4}{9} \Delta_0$$

 $=\frac{2}{3}\left(\frac{\Delta_0}{6}\right)$

Therefore, for four ligand,

The relationship of crystal field splitting energy for octahedral($\Delta 0$) and tetrahedral (Δt) complexes is-

 $\Delta t = \frac{4}{9} \Delta_0$

Q13. How does the magnitude of Δ_0 decide the actual configuration of d orbitals in a coordination entity?

Answer. If Δ_0 is greater than the pairing energy, electrons get paired in lower energy d-orbitals giving a low spin complex. On the other hand, if Δ_0 is, is less than the pairing energy, electrons occupy higher energy d-orbitals giving a high spin complex.

Q14. Explain the violet colour of $[Ti(H_2O)_6]^{3+}$ complex on the basis of the crystal field theory?

Answer. $[Ti(H_2O)_6]^{3+}$ is an octahedral complex. The oxidation state of Ti is +3 with the coordination number 6.

Its outer electronic configuration is $3d^1$, which means that it has one unpaired electron. This unpaired electron is excited from t_{2g} level to e_g level by absorbing yellow light and hence appears violet coloured.

Q15. Based on crystal field theory, write the electronic configuration of d⁴ in terms of t_{2g} and e_g in an octahedral field when $\Delta 0 > P$.

Answer. The magnitude of Δ_0 decides the actual configuration of d-orbitals with the help of mean pairing energy.



If $P > \Delta_{0,}$ then pairing of electrons does not occur, and electrons enter the higher energy orbitals and thus form high spin complexes due to weak-field ligands. Therefore, one electron enters in e_g orbital and 3 electrons in t_{2g} with configuration $t_{2g}^3 e_g^1$.

Practise Questions on Crystal Field Theory

Q1. How many unpaired electrons are there in a strong field iron(II) octahedral complex?

- a.) 0
- b.) 1
- c.) 2
- d.) 4

Correct Answer- (a.) 0

Q2. Strong field ligands such as CN⁻:

- a.) usually produce high spin complexes and small crystal field splittings.
- b.) usually produce low spin complexes and small crystal field splittings.
- c.) usually produce low spin complexes and high crystal field splittings.
- d.) usually produce high spin complexes and high crystal field splittings.

Correct Answer- (c.) usually produce low spin complexes and high crystal field splittings.

Q3. The hexaaquo manganese (II) ion contains five unpaired electrons while the hexacyano ion contains only one unpaired electron. Explain using Crystal Field Theory.

Answer.

[Mn(H ₂ O) ₆] ²⁺	[Mn(CN) ₆] ^{4–}
Mn is in the +2 oxidation state.	Mn is in the +2 oxidation state.
The electronic configuration is d⁵.	The electronic configuration is d ⁵ .
The crystal field is octahedral. Water is a	The crystal field is octahedral. Cyanide is a
weak field ligand. Therefore, the	strong field ligand. Therefore, the
arrangement of the electrons in [Mn(H ₂ O) ₆] ²⁺	arrangement of the electrons in [Mn(CN) ₆] ^{4–}
is $t_{2a}^{3}e_{a}^{2}$.	ist _{2a} ⁵ e _a ⁰ .

Hence, the hexaaquo manganese (II) ion has five unpaired electrons, while the hexacyano ion has only one unpaired electron.

Q4. Why does Co²⁺ readily oxidise to Co³⁺ in complexes?

Answer. In the presence of a weak ligand, Co^{2+} (d⁷) has electronic configuration $t_{2g}^{5}e_{g}^{2}$. There are three unpaired electrons.



In the presence of a strong ligand, the difference in energy between t_{2g} and e_g levels increases. So, out of three unpaired electrons, two become paired, and there remains only one unpaired electron at the e_g level. This electron from higher energy, e_g level is easily lost to form Co³⁺ ion having stable configuration t_{2g}^{-6} with high CFSE. Thus Co²⁺ is easily oxidised to Co³⁺ in the presence of a strong ligand.

Q5. What is the Difference Between VBT and CFT?

Answer. VBT is an abbreviation for valence bond theory. CFT is an abbreviation for crystal field theory. The main difference between VBT and CFT is that VBT explains the mixing of orbitals while CFT explains the splitting of orbitals.



