Tutorial: Discussion of questions with answers on MOT and CFT

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Calculation of CFSE for few octahedral and tetrahedral complexes

Step-1: Determine the oxidation state of central metal ion

Step-2: Determine the number of d-electrons present in the central metal cation

Step-3: Consider whether it is octahedral or tetrahedral complex

Step-4: If it is octahedral complex, then decide about the weak field or strong field cases leading to high spin or low spin complex, respectively

Step-5: If it is tetrahedral complex, then consider only high spin complex case

Step-6: Once the splitting of d-electrons among t_{2g} and e_g is decided, the CFSE can be determined by considering the case of octahedral or tetrahedral complex.

Calculation of CFSE under weak field and strong field cases

	Weak field			Strong field		
d^n	Configu-ration	Unpaired e⁻s	CFSE	Confi-guration	Unpaired e⁻s	CFSE
d^1	$t_{2g}^1 e_g^0$	1	**-0.4 Δ_o**	$t_{2g}^1 e_g^0$	1	**-0.4 Δ_o**
d^2	$t_{2g}^2 e_g^0$	2	**-0.8 Δ_o**	$t_{2g}^2 e_g^0$	2	**-0.8 Δ_o**
d^3	$t_{2g}^3 e_g^0$	3	**-1.2 Δ_o**	$t_{2g}^3 e_g^0$	3	**-1.2 Δ_o**
d^4	$t_{2g}^3 e_g^1$	4	**-0.6 Δ_o**	$t_{2g}^4 e_g^0$	2	-1.6 Δ_o
d^5	$t_{2g}^3 e_g^2$	5	**0 Δ_o**	$t_{2g}^5 e_g^0$	1	**-2.0 Δ_o**
d^6	$t_{2g}^4 e_g^2$	4	**-0.4 Δ_o**	$t_{2g}^6 e_g^0$	0	**-2.4 Δ_o**
d^7	$t_{2g}^5 e_g^2$	3	**-0.8 Δ_o**	$t_{2g}^6 e_g^1$	1	**-1.8 Δ_o**
d^8	$t_{2g}^6 e_g^2$	2	**-1.2 Δ_o**	$t_{2g}^6 e_g^2$	2	**-1.2 Δ_o**
d^9	$t_{2g}^6 e_g^3$	1	**--0.6 Δ_o**	$t_{2g}^6 e_g^3$	1	**0.6 Δ_o**
d^{10}	$t_{2g}^6 e_g^4$	0	**0 Δ_o**	$t_{2g}^6 e_g^4$	0	**0.0 Δ_o**

Qn **1**. In the molecular orbital diagram of NO molecule, how many unpaired electrons would be present?

a) three

b) Two

c) Zero

d) One

2. Gold has a work function of 5.1 eV. Find the cut off wavelength for the photoelectric effect**.**

a) 286 nm

b) 243 nm

c) 186 nm

d) 267 nm

3. Bond Order of CO, B2, F2 respectively are _____

a) +3, +2, +1

b) +2, +3, +1

c) +3, +1, +1

d) +2, +2, +1

4. Which of the following is the most paramagnetic in nature?

a) N_2

b) BC

c) NO

d) O2

5. The highest occupied pi molecular orbital of butadiene will have how many nodes?
a) 2
b) 1
c) 0
d) 3

6. Among the complexes [Cr(NH3)6]3+ and [V(NH3)6]2+ which one possesses larger value of Δ_o ?

7. Calculate the CFSE values for d3 and d8 configurations of weak field octahedral complexes.
a) 0 Δo and -1.2 Δo
b) 1.2 Δo and -1.2 Δo
c) -1.2 Δo and -1.2 Δo
d) -1.2 and 0

8. Calculate the CFSE values for d4 and d7 configurations of high spin tetrahedral complexes.
a) 0 Δo and 0 Δo
b) 0.18 Δo and 0.54 Δo
c) -0.54 Δo and -0.18 Δo
d) -0.18 Δo and -0.54 Δo

9. Calculate the magnetic moment of $Na_3[FeF_6]$
a) 4.9 BM
b) 5.92 BM, c) 0 BM, d) 2.80 BM