Crystal Field Stabilization Energy

In octahedral complexes, the *d*-orbitals of the central metal cation are split into two sets of diff these two energy level (t_{2g} of lower energy and e_g of higher energy). The energy difference between these two is Δ_0 or 10 Dq. The energy of t_{2g} set is lowered by 0.4 Δ_0 (= 4 Dq) while the energy of e_g s increased by 0.6 Δ_0 (= 6 Dq) relative to the hypothetical energy state. In other words we can say three of the *d* orbitals (i.e. t_{2g} orbitals) are stabilised by 0.4 Δ_0 per electron and two of the *d*-orbitals (e_g orbitals) are destabilised by 0.6 Δ_0 per electron. Thus energy of each electron in t_{2g} orbitals decre by – 0.4 Δ_0 while in e_g orbitals increases by + 0.60 Δ_0. – and + signs indicate decrease and increas the energy respectively.

For d^1 case, the electron occupies a t_{2g} orbitals, which has an energy of – 0.4 Δ_0 relative to barycentre of the *d*-orbitals. The complex can thus be said to be stabilized to the extent of 0.4 compared to the barycentre. This quantity is termed as crystal field stabilization energy.

Thus for d^1 complex, electronic configuration is $t_{2g}^1\ e_g^0$

$$\text{CFSE} = -0.4 \times 1\ \Delta_0 = -0.4\ \Delta_0$$

For d^2 complex, electronic configuration is $t_{2g}^2\ e_g^0$

$$\text{CFSE} = -0.4 \times 2\ \Delta_0 = -0.8\ \Delta_0$$

For d^3 complex, electronic configuration is $t_{2g}^3\ e_g^0$

$$\text{CFSE} = -0.4 \times 3\ \Delta_0 = -1.2\ \Delta_0$$

For d^4 high spin complex, electronic configuration is $t_{2g}^3\ e_g^1$

$$\text{CFSE} = [-0.4 \times 3 + 0.6 \times 1]\ \Delta_0 = -0.6\ \Delta_0$$

Thus, in case of an octahedral complex with the configuration $t_{2g}^p\ e_g^q$, the crystal field stabilisation given by,

$$\text{CFSE} = [-0.4\ \text{p} + 0.6\ \text{q}]\ \Delta_0$$

The CFSE may be defined as "The net energy of a complex which stabilised the complex relative to th hypothetical energy state." CFSE is a measure of the net energy of occupation of the *d*-orbital relative their mean energy (or hypothetical energy).

CFSE for d^1 to d^{10} for HS and LS octahedral complexes is given in the table:

	Weak field high spin		Strong field low spin	
d^n	Configuration	CFSE	Configuration	CFSE
d^1	t_{2g}^1	$-0.4 \times 1\ \Delta_0 = -0.4\ \Delta_0$	t_{2g}^1	$-0.4 \times 1\ \Delta_0 = -0.4\ \Delta_0$
d^2	t_{2g}^2	$-0.4 \times 2\ \Delta_0 = -0.8\ \Delta_0$	t_{2g}^2	$-0.4 \times 2\ \Delta_0 = -0.8\ \Delta_0$
d^3	t_{2g}^3	$-0.4 \times 3\ \Delta_0 = -1.2\ \Delta_0$	t_{2g}^3	$-0.4 \times 3\ \Delta_0 = -1.2\ \Delta_0$
d^4	$t_{2g}^3\ e_g^1$	$[-0.4 \times 3 + 0.6 \times 1]\ \Delta_0 = -0.6\ \Delta_0$	t_{2g}^4	$-0.4 \times 4\ \Delta_0 = -1.6\ \Delta_0$
d^5	$t_{2g}^3\ e_g^2$	$[-0.4 \times 3 + 0.6 \times 2]\ \Delta_0 = 0.0\ \Delta_0$	t_{2g}^5	$-0.4 \times 5\ \Delta_0 = -2.0\ \Delta_0$
d^6	$t_{2g}^4\ e_g^2$	$[-0.4 \times 4 + 0.6 \times 2]\ \Delta_0 = -0.4\ \Delta_0$	t_{2g}^6	$-0.4 \times 6\ \Delta_0 = -2.4\ \Delta_0$
d^7	$t_{2g}^5\ e_g^2$	$[-0.4 \times 5 + 0.6 \times 2]\ \Delta_0 = -0.8\ \Delta_0$	$t_{2g}^6\ e_g^1$	$[-0.4 \times 6 + 0.6 \times 1]\ \Delta_0 = -1.8\ \Delta_0$
d^8	$t_{2g}^6\ e_g^2$	$[-0.4 \times 6 + 0.6 \times 2]\ \Delta_0 = -1.2\ \Delta_0$	$t_{2g}^6\ e_g^2$	$[-0.4 \times 6 + 0.6 \times 2]\ \Delta_0 = -1.2\ \Delta_0$
d^9	$t_{2g}^6\ e_g^3$	$[-0.4 \times 6 + 0.6 \times 3]\ \Delta_0 = -0.6\ \Delta_0$	$t_{2g}^6\ e_g^3$	$[-0.4 \times 6 + 0.6 \times 3]\ \Delta_0 = -0.6\ \Delta_0$
d^{10}	$t_{2g}^6\ e_g^4$	$[-0.4 \times 6 + 0.6 \times 4]\ \Delta_0 = 0.0\ \Delta_0$	$t_{2g}^6\ e_g^4$	$[-0.4 \times 6 + 0.6 \times 4]\ \Delta_0 = 0.0\ \Delta_0$