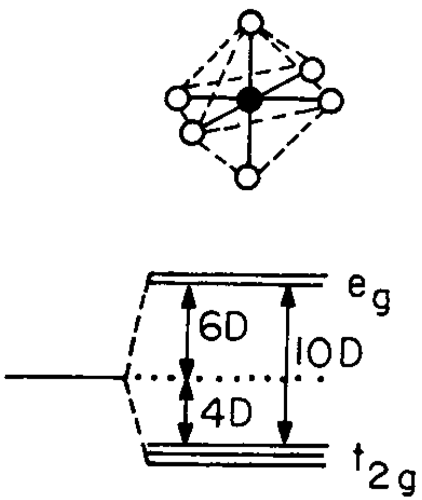
# Crystal field for 3d ions : cubic crystal field

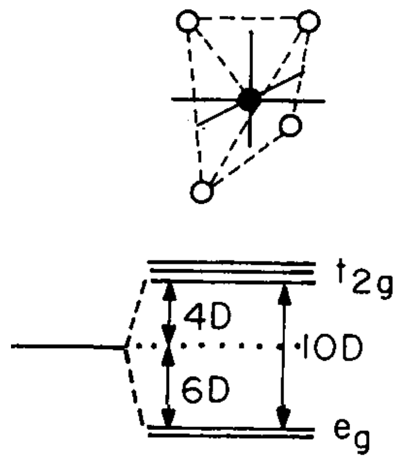
**Crystal field potential:** $V_c = V_0(x^4 + y^4 + z^4 - 3/5r^4)$

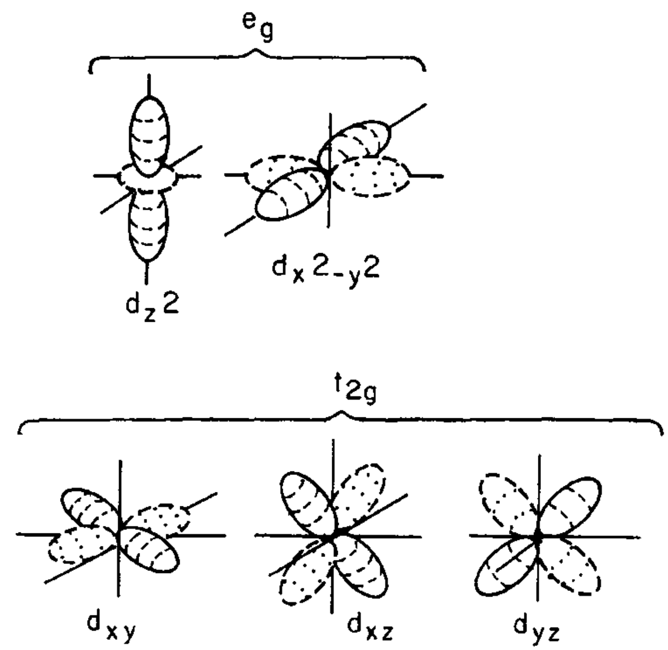
**d orbitals are splitted in 2 groups: $e_g$ and $t_{2g}$; 2 cases:**

## octahedral

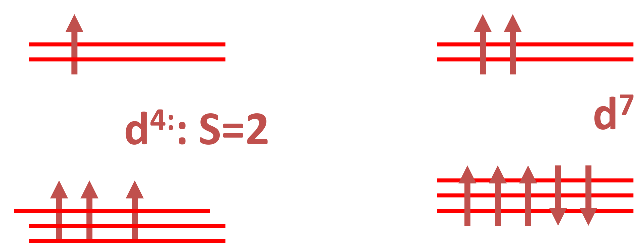



## tetrahedral




**Filling of the d-orbitals following 1st Hund's rule (S maximum)**



$d^4$: S=2

$d^7$ : S=3/2

# Quenching of orbital magnetic moment:

Wave functions of $e_g$ states: $\frac{1}{\sqrt{2}}(Y_2^2 + Y_2^{-2})$ and $Y_2^0$

No orbital magnetism:

$$\langle e_g^1 | L_\alpha | e_g^2 \rangle = 0, \alpha = x, y, z$$

$t_{2g}$ states: $\frac{1}{\sqrt{2}}(Y_2^2 - Y_2^{-2}), \frac{1}{\sqrt{2}}(Y_2^1 - Y_2^{-1})$, and $\frac{1}{\sqrt{2}}(Y_2^1 + Y_2^{-1})$

Diagonal matrix elements of $L_\alpha$ vanish, only off-diagonal elements:
$\Rightarrow$« reduced » orbital moment

In cubic symmetry orbital magnetism is either quenched ($e_g$) or reduced ($t_{2g}$):
L is not given by Hund's rule

Spin-orbit coupling is a smaller effect, acting mainly in $t_{2g}$ states