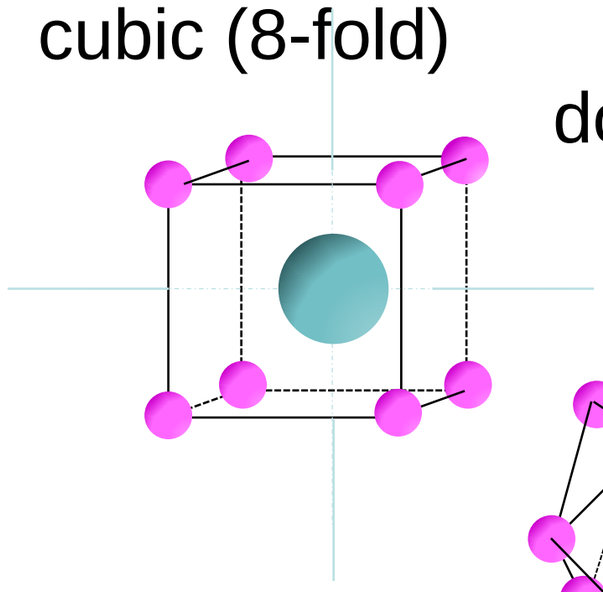
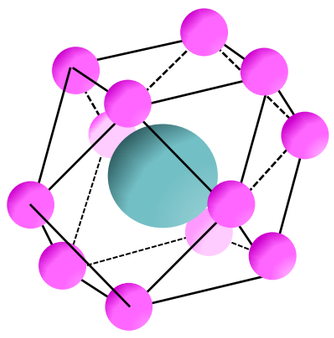
Energy splitting of 3d-orbitals in crystal fields

CaF_2	II:VI; III:V	MgO; NaCl

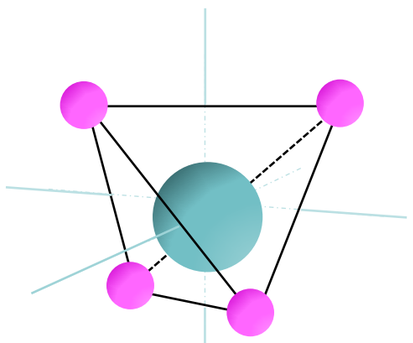
cubic (8-fold)



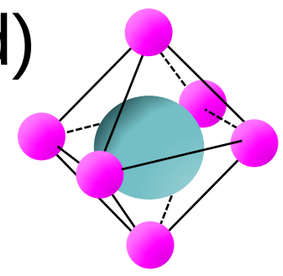
dodecahedral (12-fold)



Tetrahedral, T_d (4-fold)



octahedral, O_h (6-fold)



$3d_{x^2-x^2}$ $3d_{z^2}$ $3d_{zx}$ $3d_{xy}$ $3d_{yz}$

$$\Delta_o : \Delta_c : \Delta_d : \Delta_t = 1 : \left(-\frac{8}{9}\right) : \left(-\frac{1}{2}\right) : \left(-\frac{4}{9}\right)$$

crystal field parameters

$(Z_L e)$ is ligant charge separated by distance R from the cation; $\langle r^4 \rangle_{3d}$ is mean value of the radial distance of 3d orbitals from nucleus

$$\Delta_o = 10D_q = \left(\frac{3}{5}\right)\left(\frac{Z_L e^2}{4\pi\epsilon_0 R^5}\right)\langle r^4 \rangle_{3d}$$