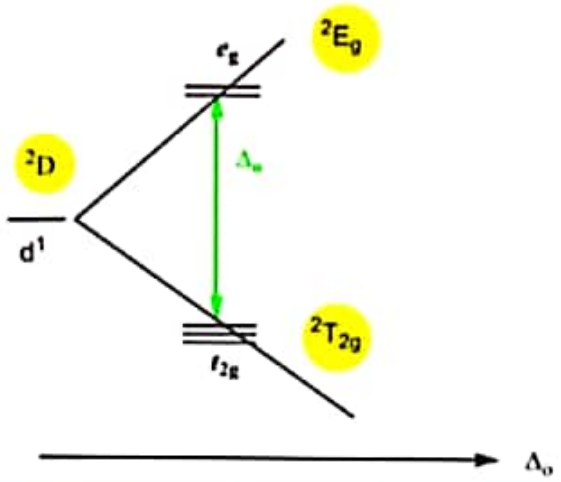
The splitting of S, P, D, F terms in an octahedral crystal field is as follows.

Atomic term	Crystal field term (in O_h symmetry)
S	A_{1g}
P	T_{1g}
D	E_g
	T_{2g}
F	A_{2g}
	T_{1g}
	T_{2g}
G	A_{1g}
	E_g
	T_{1g}
	T_{2g}

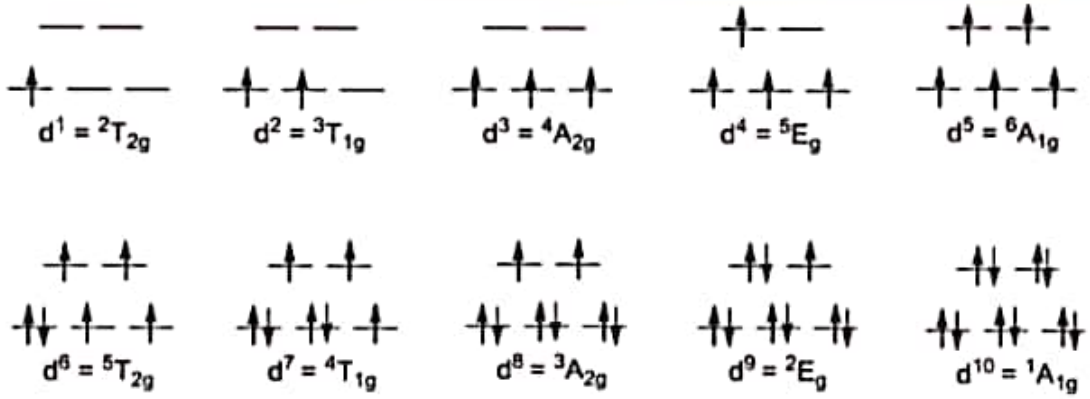
Example: The splitting of the ^2D term in an octahedral crystal field



General points:
- Spin multiplicity is not perturbed by the ligand field
- In centrosymmetric complexes, all split terms are labeled g (gerade)
- g,u symbols not applicable in non-centrosymmetric complexes
- ground terms can be taken from the Tanabe Sugano diagrams
- S and P terms are not split by an octahedral crystal field

Order of energies of crystal field terms

a) Determination of the ground terms



When there is a single unpaired e⁻ in the t_{2g} orbitals, $(t_{2g})^1$, the symmetry of the corresponding term is the same as that of the orbital and written in capitals (T_{2g}).

When there are two unpaired electrons in t_{2g} orbitals, three occupations are possible. Therefore it is a triply degenerate term, T. It is not possible to know a priori if it is a T_{1g} or T_{2g} term. It is necessary to perform group theoretical calculations (symmetry descent method). It turns out that the $^3T_{1g}$ term is the ground term.

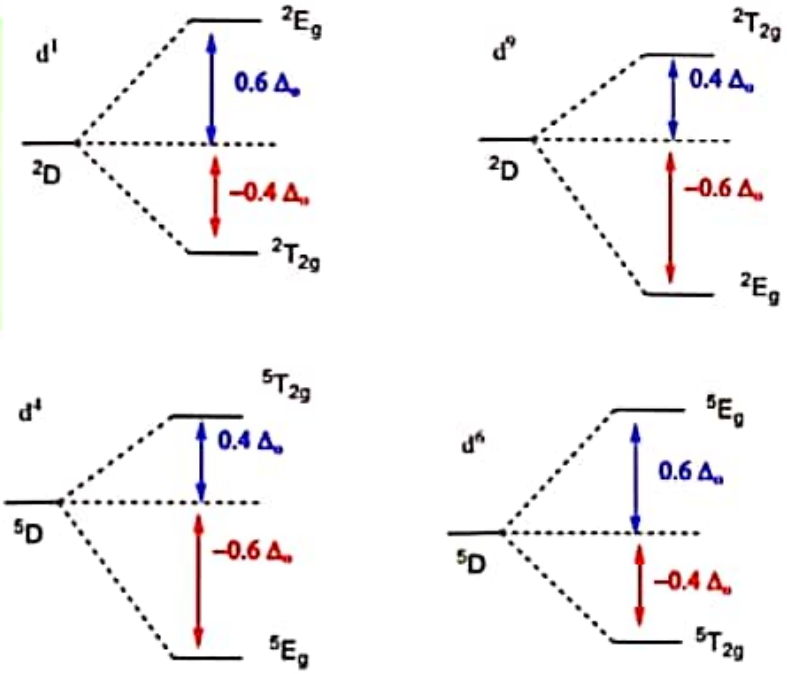
The other ground states are determined in a similar fashion (but this is out of the scope of the present lecture).

Order of energies of crystal field terms

b) Determination of the energies of the upper ligand field terms

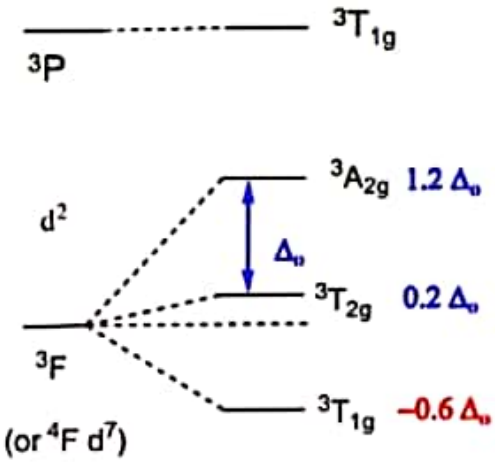
In case of d^1,d^4,d^6 and d^9 systems, the energies of the upper levels are relatively easy to calculate (from the degeneracies of the terms)

T: triply degenerate
E: doubly degenerate term

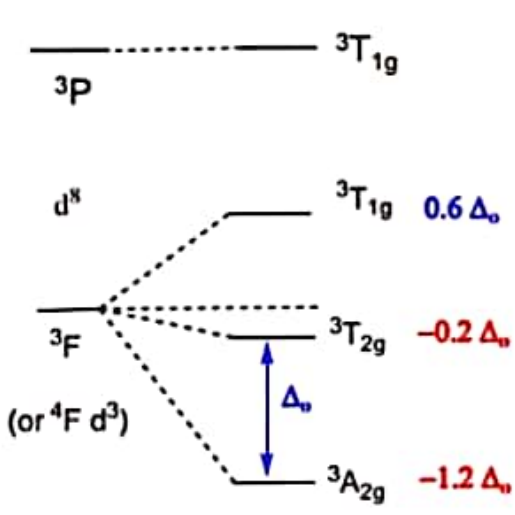


Energies of the crystal field terms: d^2, d^3, d^7, d^8 configuration

- are more difficult to calculate (beyond the scope of this lecture)
- only the results are given here (splitting of the ground terms) (without consideration of the configuration interaction)



d²



d⁸