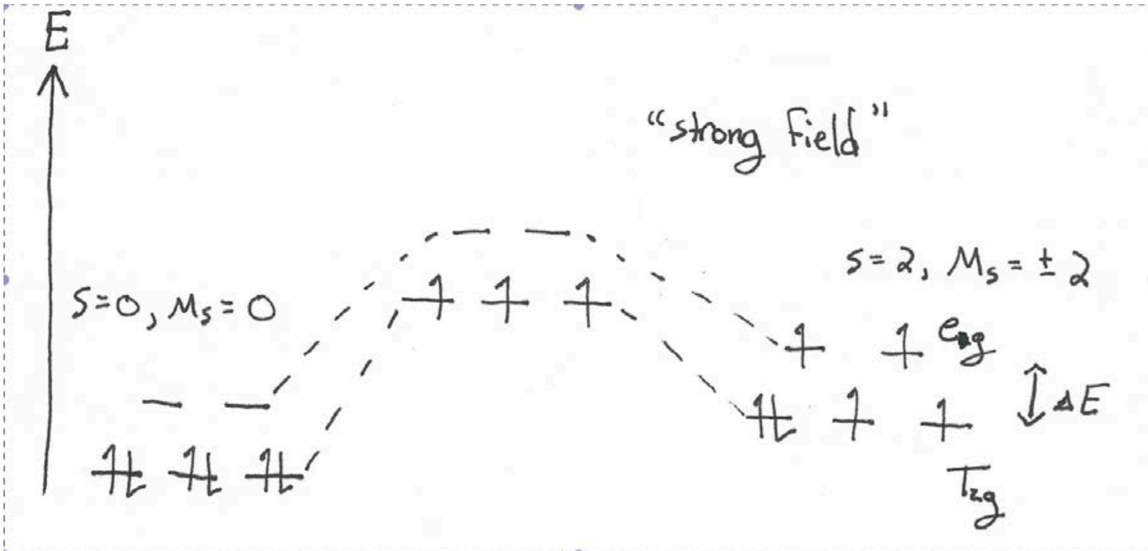
Homework H31 Solution

1. **Turn in** The species $[Co(NH_3)_6]^{3-}$ has spin S=0. Draw a diagram showing how the low and high spin cases differ in MO theory when the last 3 electrons are filled in. [Hint: when you fill in the last three electrons, the orbital energies of the E_g and T_{2g} orbitals actually shift around, as discussed in class for CoF_6^{6-}.]

Solution:



As you can see in the diagram above, the S=0 (low spin) case is lower in energy than the S=2 (high spin) case. We are told that the species $[Co(NH_3)_6]^{3-}$ has spin S=0, and since we know that chemical species adopt the lowest energy configuration possible under a set of given conditions, this implies that the S=0 state is the state of lowest energy.

We know from our treatment of the hydrogen atom that the five d orbitals of Cobalt are degenerate, but this degeneracy is removed in crystal field theory (which we will not talk about in this solution; the details are immaterial for our purpose here, we simply need to know that there *is* a removal of degeneracy). This gives rise to the E_g and T_{2g} orbitals, separated by an energy ΔE as shown in the above diagram. In a "weak field", the ΔE is small, and while it takes energy to put electrons in the E_g orbitals because they are higher in energy than the T_{2g} orbitals, there is also electron repulsion energy saved by maximizing spin and not pairing electrons. So in the weak field/small ΔE case, the net energy of the high spin case is lower and in the "strong field"/large ΔE, the net energy of the low spin case is lower.

Note in the above figure we drew the low spin case 1-electron orbitals clearly lower in energy than the high spin case 1-electron orbitals. However, even if the orbital energies of the low spin case at the same or even slightly higher energy than the high spin case, the low spin case would still 'win.' The high spin case only 'wins' if the small DE splitting makes up for electron repulsion.