Summary of Results useful for Deriving Atomic Term Symbols

Detailed Examples are provided in the textbook and lecture

1) **closed shells** have L=0 and S=0

2) **non-equivalent electrons**: easy! find all possible values of L and S using the vector sum rules, combine them to form the terms

3) **equivalent electrons**: this is best demonstrated by example as they must obey the Pauli principle. Write down a table with each line representing a Slater determinant for a particular value of m_l and m_s for each electron. Deduce the term due to the largest L value and work your way through. Double check you have accounted for all states. The number of state in a term is (2L+1)(2S+1), make sure you have accounted for all states when you are done.

4) **'holes' in shells** have the same terms as electrons in shells (p^5 has the same terms as p^1, p^4 has the same as p^2, d^9 the same as d^1, etc.)

5) **configs. with both equivalent and non-equivalent electrons:** first separately find the terms for the equivalent and non-equivalent electrons. Then take all possible combinations of L and S values from pair-wise combinations from these two sets of terms.

6) Use Hund's rules to determine the lowest energy term (See text).

Hund’s (Empirical) Rules:

1) The state with the largest S is the most stable (and stability [usually] decreases with decreasing S)

aka-UNPAIRED SPINS ARE FAVORED

2) For states with the same S the largest L state has the lowest E

3) for < ½ filled orbitals smallest J is most stable (“regular”)

for > ½ filled orbitals largest J is most stable (“inverted”)