2.11: Term Symbols

Term symbols are a shorthand method used to describe the energy, angular momentum, and spin multiplicity of an atom in any particular state. From a spectroscopic perspective, we need to know the values for the various types of angular momenta. Term symbols provide three pieces of information

- Total orbital angular momentum, L
- Multiplicity of the term, $2S+1$
- Total angular momentum, J

$$^{2S+1}L_J$$

Total Angular Momentum

$$L = l_1 + l_2 + l_3 + \ldots$$

- Maximum L is $l_1 + l_2$
- Minimum L is $|l_1 - l_2|$

$$\begin{array}{lccccc} \text{L:} & 0 & 1 & 2 & 3 & 4 \\ & \text{S} & \text{P} & \text{S} & \text{F} & \text{G} \end{array} \tag{2.11.1}$$

Spin Multiplicity

We can also determine the multiplicity options using a Clebsch-Gordan series

$$S = ½ + ½, ½ - ½$$

For two electron system S=0 and the spin multiplicity given by

$$2S+1$$

- For $S = 1$ (two unpaired electrons): $2S+1 = 3$ This is called a **triplet** state
- For $S = 0$ (no unpaired electrons): $2S+1 = 1$ This is called a **singlet** state

Total Angular Momentum

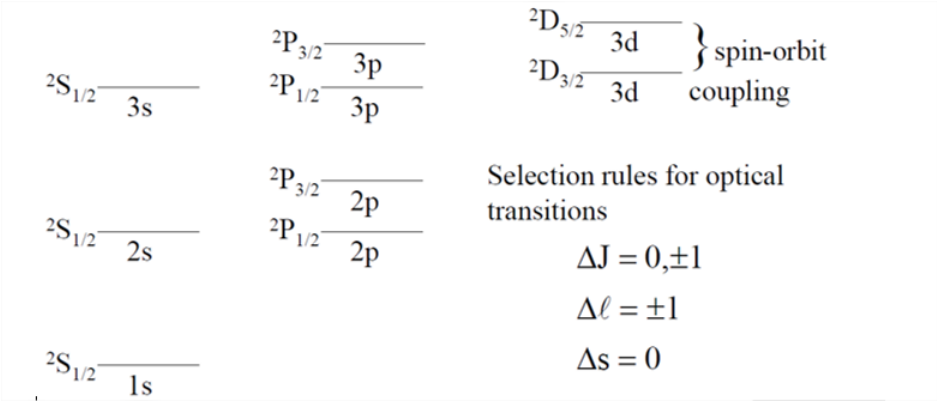
Permitted values of J again, given by a Clebsch-Gordon series

$$J = L+S, L+S-1, L+S-2 \ldots . |L-S|$$

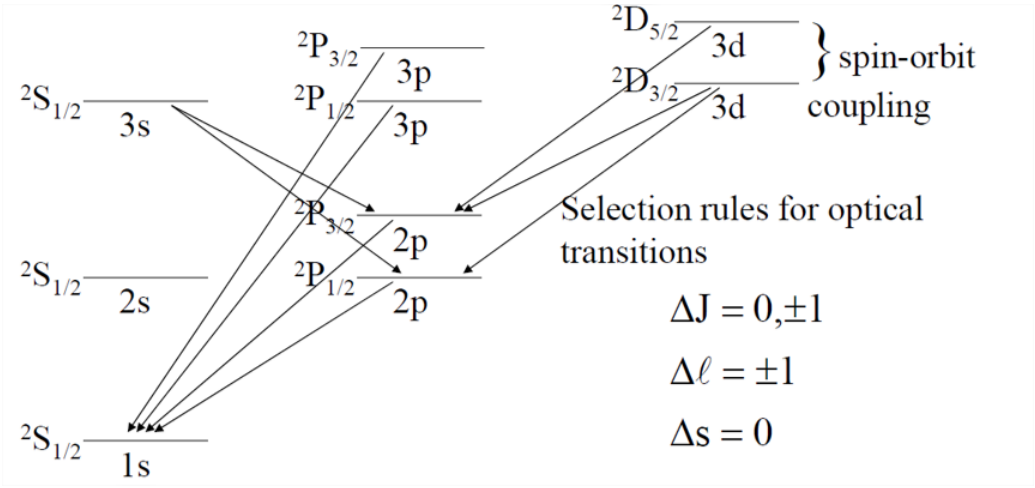
Example 2.11.1

- *H($1s^1$) : ground state term symbol is $^2S_{1/2}$. Hence only one possible state for this "configuration"*
- *He($1s^2$) : Ground state term symbol is $^1S_0$. Hence only one state possible for this "configuration"*
- *Now, what about the excited hydrogen atom*. For case with L =1, S = ½ J = 1 + ½ or 1 - ½ the term symbols are $^2P_{3/2}$ and $^2P_{1/2}$

A portion of the hydrogen atom transition level diagram for optical spectra then, will look like



And with allowed transitions:



What about Ne? For $2p^6$ configuration, only one set of possible values.

$$M_L = m_1 + m_2 + m - 3 + m - 4 + m_5 + m_6 = 1 + 1 + 0 + 0 + (-1) + (-1) = 0$$

And in this case we also have

$S = |M_s| = m_{s1} + m_{s2} + m_{s3} + m_{s4} + m_{s5} + m_{s6}$

$= ½-½ + ½-½ + ½-½ = 0$

Thus, term is ^1S_o. **We will find this to be true for ANY filled subshell**. More complicated terms occur with unfilled shells (e.g., excited states). How to dictate energy levels of these states? Use Hund's rules:

1. State with the **largest** value of S is most stable and stability decreases with decreasing S.

2. For states with same values of S, the state with the **largest** value of L is the most stable.

3. If states have same values of L and S then, for a subshell that is less than half filled, state with **smallest** J is most stable; for subshells that are more than half filled, state with **largest** value of J is most stable.

Example 2.11.1

Example: Consider the terms ^3D, ^3P, ^3S, ^1D, ^1P, ^1S to describe the same electron distribution in an atom. In terms of stability we can rank these terms as:

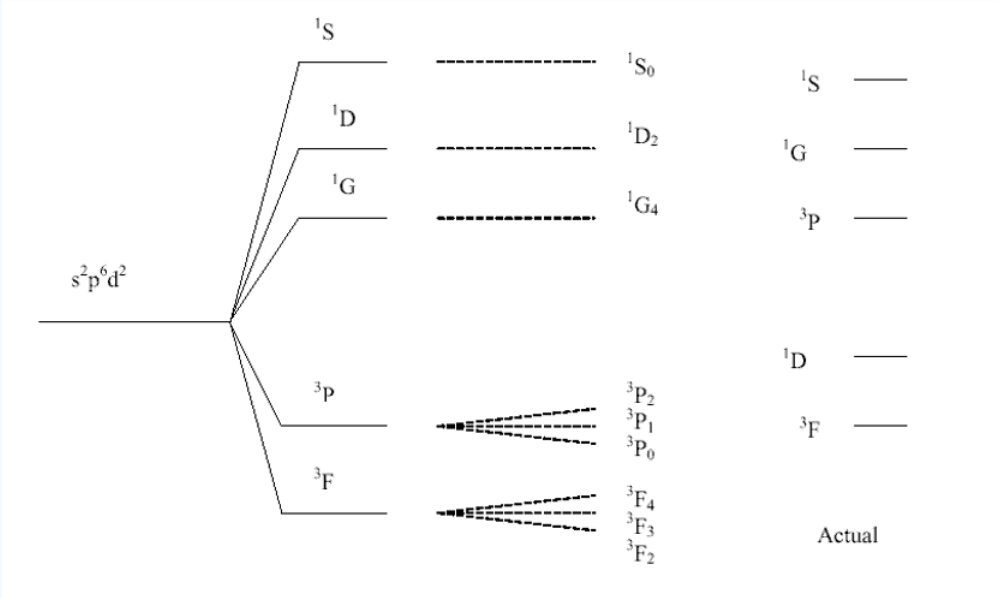
$^1S > {}^1P > {}^1D > {}^3S > {}^3P > {}^3D$ Most stable

Given that the ^3D states are most stable, which of these terms correspond to the most stable state? Since the two p subshells are less than half filled, we would predict that the 3D1term corresponds to the most stable state! Simple approach for finding the ground state term symbol for any atom:

- Find maximum value of S consistent with the Pauli Exclusion Principle: S = S_{max}.
- For S = S_{max}, find the maximum value of L consistent with the Pauli Exclusion Principle: L = L_{max}.
- Apply Hund's Rules to find J for most stable state.

Example 2.11.2

He($1s^1 2s^1$): An Excited State Configuration
Terms: $^1S_0$, $^3S_1$
{ There is no $^3S_0$ nor $^3S_{-1}$ Term }



Configuration	Terms
p^1, p^5	^2P
p^2, p^4	^3P, ^1D, ^1S
p^3	^4S, ^2P, ^2D
d^1, d^9	^2D
d^2, d^8	^3P, ^3F, ^1S, ^1D, ^1G
d^3, d^7	^2P, ^2D, ^2D, ^2F, ^2G, ^2H, ^4P, ^4F
d^4, d^6	^1S, ^1S, ^1D, ^1D, ^1F, ^1G, ^1G, ^1I, ^3P, ^3P, ^3D, ^3F, ^3F, ^3G, ^3H, ^5D
d^5	^2S, ^2P, ^2D, ^2D, ^2D, ^2F, ^2F, ^2G, ^2G, ^2H, ^2I, ^4P, ^4D, ^4F, ^4G, ^6S