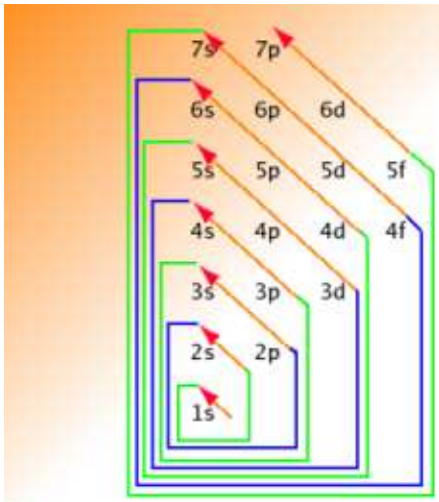

$^{2S+1}L_J$

A quick guide

Hund's Rules, and a binary simplification.

- States with larger S lie lower
- For an S state, the higher the L, the lower the energy
- For any L and S, if the shell is less than half-filled, the lower state has $J = |L - S|$, else the lower state is $J = L + S$.

Z	*n* - *l* - *shell*	Shell	Code
1	$001 - 000 - \oslash$	$(1s)$	$^2S_{1/2}$
2	$001 - 000 - \otimes$	$(1s)^2$	$^1S_0$
3	$010 - 000 - \oslash$	$(He)(2s)$	$^2S_{1/2}$
4	$010 - 000 - \otimes$	$(He)(2s)^2$	$^1S_0$
5	$010 - 001 - \circ\circ\oslash$	$(He)(2s)^2(2p)$	$^2P_{1/2}$
6	$010 - 001 - \circ\oslash\oslash$	$(He)(2s)^2(2p)^2$	$^3P_0$
7	$010 - 001 - \oslash\oslash\oslash$	$(He)(2s)^2(2p)^3$	$^4S_{3/2}$
8	$010 - 001 - \oslash\oslash\otimes$	$(He)(2s)^2(2p)^4$	$^3P_2$
9	$010 - 001 - \oslash\otimes\otimes$	$(He)(2s)^2(2p)^5$	$^2P_{3/2}$
10	$010 - 001 - \otimes\otimes\otimes$	$(He)(2s)^2(2p)^6$	$^1S_0$
11	$011 - 000 - \oslash$	$Ne(3s)$	$^2S_{1/2}$
12	$011 - 000 - \otimes$	$Ne(3s)^2$	$^1S_0$

Binary addition is based on powers of 2:

$$\underbrace{1}_{2^2}\ \underbrace{1}_{2_1}\ \underbrace{0}_{2_0} = 1\times 4 + 1\times 2 + 0\times 1 = 5$$

A binary system can be used to identify hydrogen:

$$\overbrace{1}^{Z} - \overbrace{001}^{n=1} - \overbrace{000}^{l=0} - \overbrace{\oslash}^{\text{Shell half-filled}} \Rightarrow (1s) : {}^2S_{1/2}$$

Here, $l = 0$ so our main label is S. There is one unpaired electron, so that our spin is 1/2, whereby we have ^2S. Finally, the shell is at least half filled, so our J is additive.

How do we account for the *total* angular momentum? Based on Hund's rule that higher l corresponds to lower energy, we consider an amendment to the system that takes account of the vectoral addition of l such that we match the convention. For any set of subshells, the center shell corresponds to zero, the rightward shells correspond to increasing levels of l, and the leftward decreasing levels from zero. Consider,for example, Sc, Z = 21, whose shells will fill as

$$\overbrace{\circ}^{-2}\ \overbrace{\circ}^{-1}\ \overbrace{\circ}^{0}\ \overbrace{\circ}^{1}\ \overbrace{\oslash}^{2} \Rightarrow L = 2$$

Mn as another example gives,

$$\overbrace{\oslash}^{-2}\ \overbrace{\oslash}^{-1}\ \overbrace{\oslash}^{0}\ \overbrace{\oslash}^{1}\ \overbrace{\oslash}^{2} \Rightarrow L = 0$$

Of course, there are exceptions such as Cr, where we would expect,

$$\overbrace{\circ}^{-2}\ \overbrace{\oslash}^{-1}\ \overbrace{\oslash}^{0}\ \overbrace{\oslash}^{1}\ \overbrace{\oslash}^{2} \Rightarrow L = 2$$

It so happens, though, that Cr works out to have $L = 0$.

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