

Tableau method for determining atomic terms illustrated for a p^2 electronic configuration

As we have discussed in Chap. 2, if we have two electrons in any one of three $2p$ orbitals and two possible spin states, we have 15 different possibilities. We can create a tableau (fancy word for a table), in which these possible electron assignments are assigned to boxes corresponding to the projection of the total angular momentum

$$M_L = m_{l1} + m_{l2}$$

and to the projection of the total spin

$$M_S = m_{s1} + m_{s2}$$

Since $-1 \leq m_l \leq +1$, and $-1/2 \leq m_s \leq +1/2$ (both in integer steps), M_L and M_S are limited to $-2 \leq M_L \leq +2$ and $-1 \leq M_S \leq +1$.

Each box in the tableau contains all possible spin-orbital product wavefunctions that correspond to the values of M_L and M_S for the particular box. Allow *only* one entry for each combination; ordering does NOT create a different entry. (This is a consequence of indistinguishability). In additional entries must be consistent with the Pauli exclusion principle in that no spin-orbital can be repeated in a particular product.

For a p^2 electronic configuration the tableau is (bars designate $m_s = -1/2$)

$M_S \setminus M_L$	2	1	0	-1	-2
1		$p_1 p_0$	$p_1 \bar{p}_{-1}$	$\bar{p}_{-1} p_0$	
0	$p_1 \bar{p}_1$	$p_1 \bar{p}_0$ $\bar{p}_1 p_0$	$p_1 \bar{p}_{-1}$ $p_{-1} \bar{p}_1$ $p_0 \bar{p}_0$	$\bar{p}_{-1} \bar{p}_0$ $\bar{p}_{-1} p_0$	$p_{-1} \bar{p}_{-1}$
-1		$\bar{p}_1 \bar{p}_0$	$\bar{p}_1 \bar{p}_{-1}$	$\bar{p}_{-1} \bar{p}_0$	

1. Select the highest value of M_S . Here this is 1. There are entries in the $M_S=1$ box, so there must exist an $S=1$ (triplet) state. The highest value of M_L in the $M_S=1$ row is 1. Thus, there is an $S=1$ (triplet) state with $L=1$. This is called a P state (because $l=1$ for a single electron is called a p state). In fact it's a *triplet P* state, denoted 3P . The value of $2S+1$ (the "multiplicity") is given as a leading superscript.

There will be nine components of this state, corresponding to the possible values of M_L (+1, 0, and -1) and M_S (+1, 0, and -1). Eliminate one product wavefunction (it doesn't matter which one) from each corresponding box

2. We are left with

$M_S \setminus M_L$	2	1	0	-1	-2
1					
0	$p_1 \bar{p}_1$	$\bar{p}_1 p_0$	$p_{-1} \bar{p}_1$ $p_0 \bar{p}_0$	$\bar{p}_{-1} p_0$	$p_{-1} \bar{p}_{-1}$
-1					

3. Only $M_S = 0$ entries are left, thus all the remaining states are singlets. Select the highest value

of M_L . Here this is 2, thus there must be a $L = 2$ state (D). Thus the state is a 1D . There will be five components of this state. Eliminate one from each appropriate box.

4. We are then left with

$M_S \setminus M_L$	2	1	0	-1	-2
1					
0			$p_0 \bar{p}_0$		
-1					

5. There is only one remaining component with $M_S = 0$ and $M_L = 0$. Thus, the remaining state is a 1S .

In conclusion, for an atom with a p^2 electron configuration (*e. g.* C, N^+ , Si ...) the allowed electronic terms (states) are 3P , 1D , and 1S . Because the Hamiltonian is independent of the orientation of the z -axes (in both coordinate space and spin space), the 9 different components of the 3P state are all degenerate, as are the 5 components of the 1D state. The 1S state has only one component, and hence is non-degenerate.