8.421 Atomic Physics I *Spring, 2020*
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Lanthanide Magnetic Moments and g-Factors

Formulas

$g_{\mathrm{J}} = 3/2 + \frac{S(S+1)-L(L+1)}{2J(J+1)}$
$\mu = g_{\mathrm{J}}\mathrm{J}$

Hund's Rules

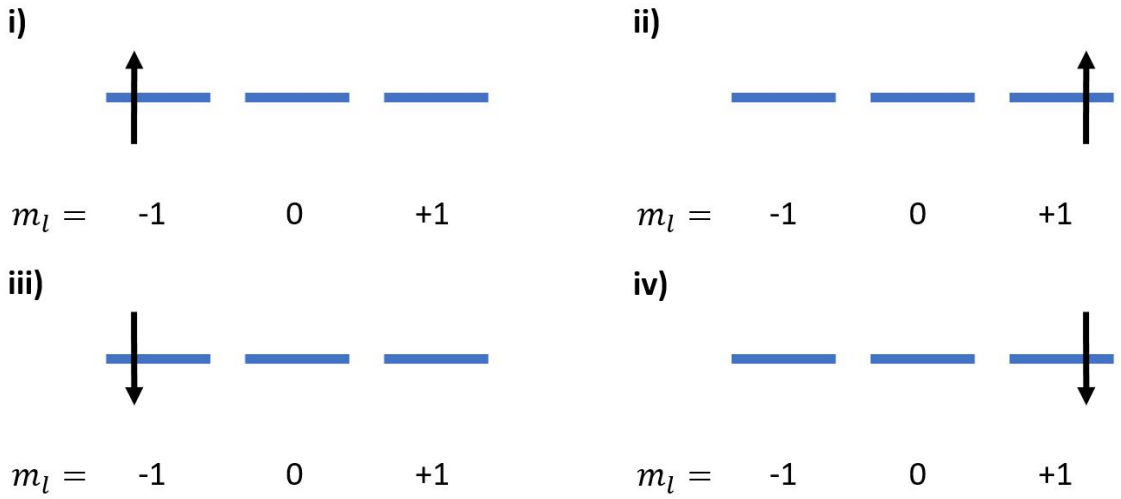
1. Maximize S
2. Maximize L
3. Account for spin-orbit coupling:

$$\mathrm{H} \propto \mathrm{L}\cdot\mathrm{S} = \frac{1}{2}\zeta(\mathrm{L,S})(\mathrm{J}^2 - \mathrm{L}^2 - \mathrm{S}^2)$$

where $\zeta(\mathrm{L,S}) = +1$ for less than half-filled shells and $\zeta(\mathrm{L,S}) = -1$ for more than half-filled shells. Therefore the ground state will minimize (maximize) J for less than (more than) half-filled shells.

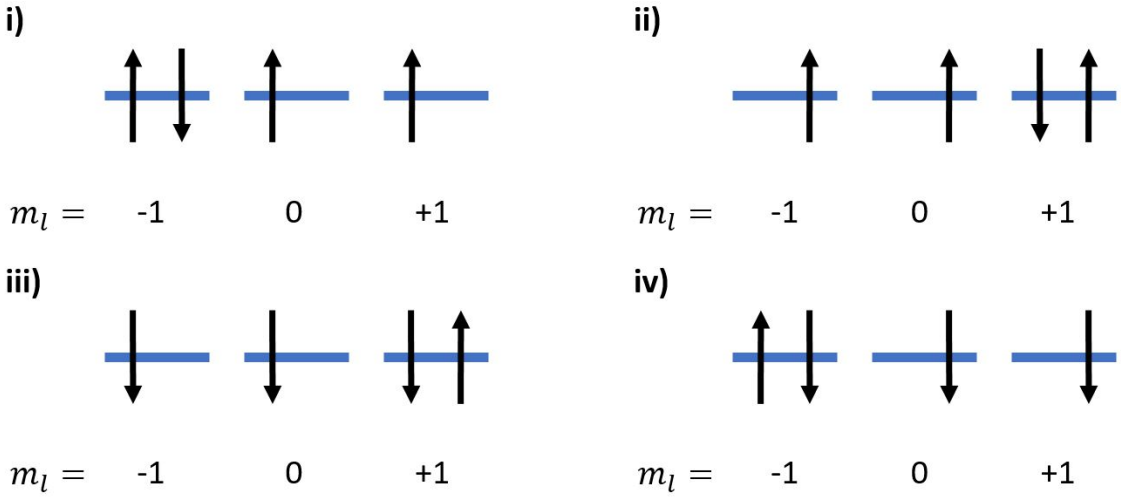
Illustration of Hund's Rules in the p-orbital

Since we must maximize L, our four options for where we could place the first electron in the p-shell are illustrated below:



To determine which of these four configurations is the ground state we must look at the spin-orbit term and minimize it: $\mathrm{L} \cdot \mathrm{S} < 0$ when L and S are anti-aligned, therefore only configurations i) and iv) are correct. When L and S are anti-aligned, J is minimized: $\mathrm{J} = |\mathrm{L} - \mathrm{S}|$.

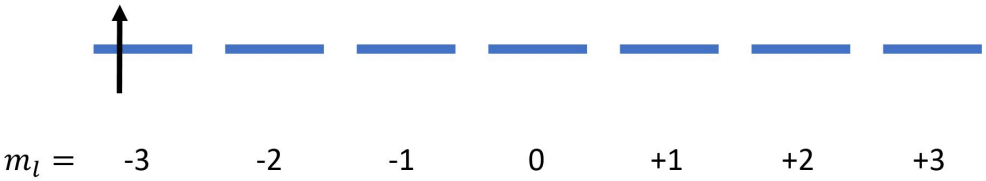
We now understand the first half of Hund's Rule 3, so let's look at the case when the shell is more than half-filled. Again, we have four possible configurations due to maximizing S and L (Hund's Rules 1 and 2):



We notice now that when the shell is more than half-filled, the electrons we add have the opposite sign compared to the first half of the shell. By looking at the four configurations we can see that for the fourth electron, $\mathrm{L} \cdot \mathrm{S} < 0$ only for ii) and iv), where the L and S of the newly added electron are anti-aligned. The newly added electron, however, is placed in an m_l that is aligned with the remaining unpaired spins! Thus we see that for more than half-filled shells, we maximize J to find the ground state: $\mathrm{J} = \mathrm{L} + \mathrm{S}$.

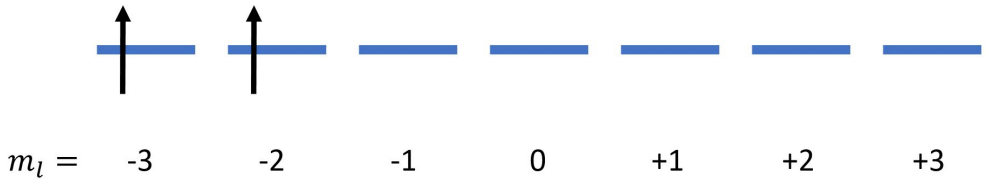
Electronic Configurations in the f-orbital

$1e^-$



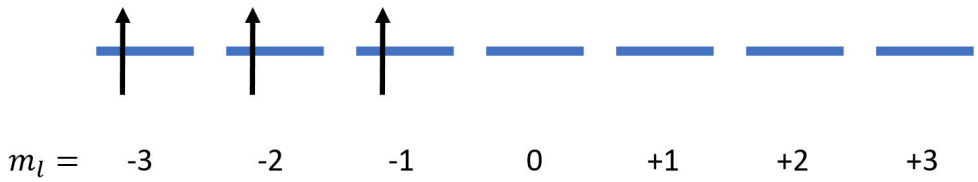
L = 3
S = 1/2
J = 3 - 1/2 = 5/2
Term Symbol: $^2F_{5/2}$
$g_J = 6/7$
$\mu = (\frac{6}{7})(\frac{5}{2}) = 15/7$

$2e^-$



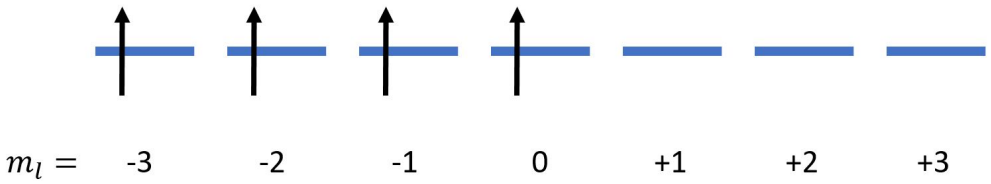
L = 3 + 2 = 5
S = 1
J = 5 - 1 = 4
Term Symbol: $^3H_4$
$g_J = 4/5$
$\mu = (\frac{4}{5})(4) = 16/5$

3e$^-$



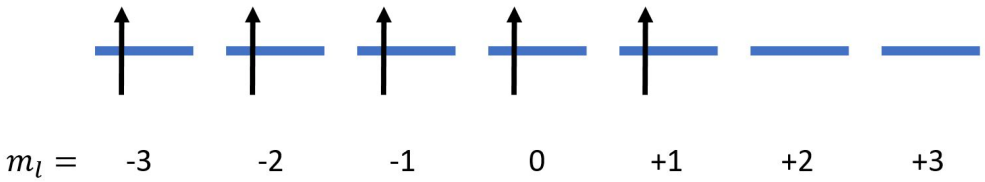
L = 3 + 2 + 1 = 6
S = 3/2
J = 6 - 3/2 = 9/2
Term Symbol: $^4I_{9/2}$
$g_J = 8/11$
$\mu = (\frac{8}{11})(\frac{9}{2}) = 36/11$

4e$^-$



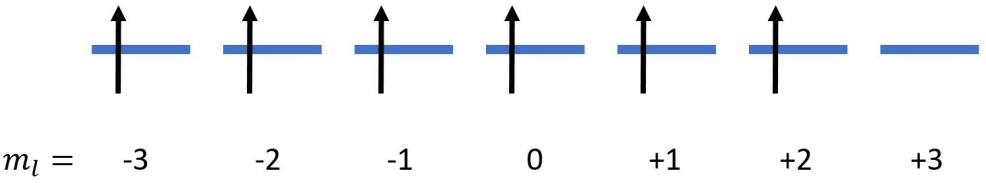
L = 3 + 2 + 1 + 0 = 6
S = 2
J = 6 - 2 = 4
Term Symbol: $^5I_4$
$g_J = 3/5$
$\mu = (\frac{3}{5})(4) = 12/5$

5e$^-$



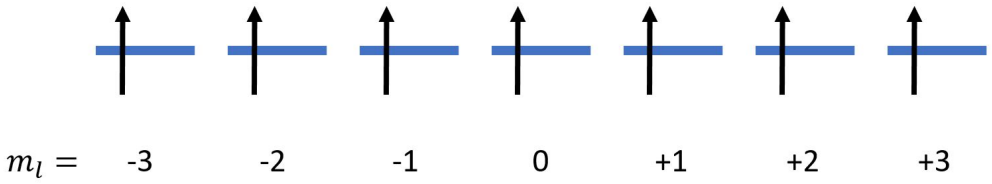
L = 3 + 2 + 1 + 0 - 1 = 5
S = 5/2
J = 5 - 5/2 = 5/2
Term Symbol: $^6H_{5/2}$
$g_J = 2/7$
$\mu = (\frac{2}{7})(\frac{5}{2}) = 5/7$

6e$^-$



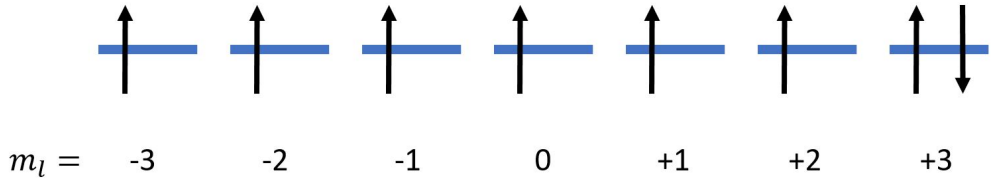
L = 3 + 2 + 1 + 0 - 1 - 2 = 3
S = 3
J = 3 - 3 = 0
Term Symbol: $^7F_0$
$g_J = 0$
$\mu = 0$

7e$^-$



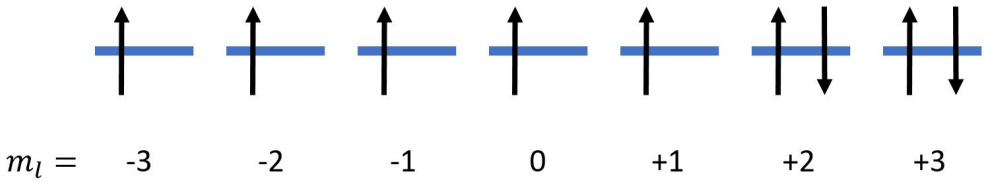
L = 3 + 2 + 1 + 0 - 1 - 2 - 3 = 0
S = 7/2
J = $|0 - 7/2| = 7/2$
Term Symbol: $^8S_{7/2}$
$g_J = 2$
$\mu = (2)(\frac{7}{2}) = 7$

8e$^-$



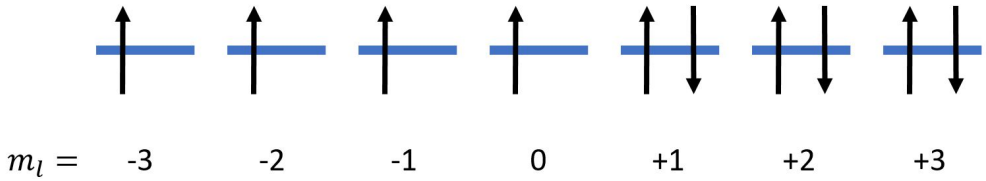
L = 3
S = 3
J = 3 + 3 = 6
Term Symbol: $^7F_6$
$g_J = 3/2$
$\mu = (\frac{3}{2})(6) = 9$

9e$^-$



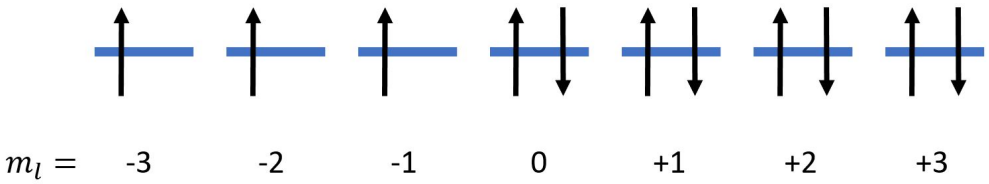
L = 3 + 2 = 5
S = 5/2
J = 5 + 5/2 = 15/2
Term Symbol: $^6H_{15/2}$
$g_J = 4/3$
$\mu = (\frac{4}{3})(\frac{15}{2}) = 10$

10e$^-$



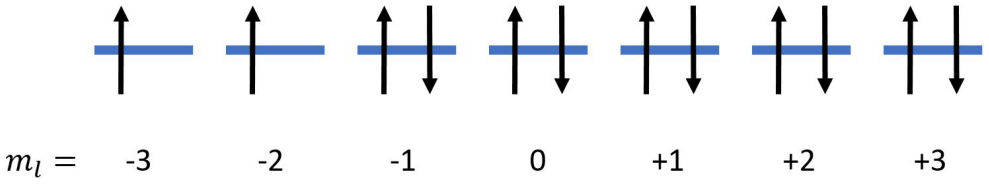
L = 3 + 2 + 1 = 6
S = 2
J = 6 + 2 = 8
Term Symbol: $^5I_8$
$g_J = 5/4$
$\mu = (\frac{5}{4})(8) = 10$

11e$^-$



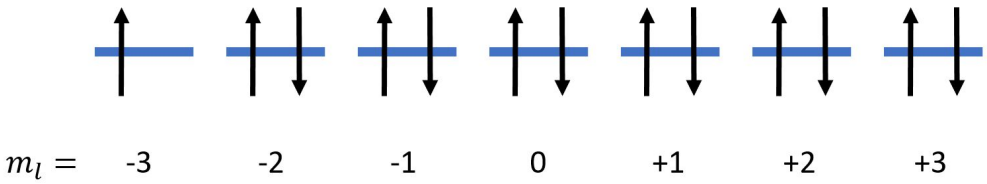
L = 3 + 2 + 1 + 0 = 6
S = 3/2
J = 6 + 3/2 = 15/2
Term Symbol: $^4I_{15/2}$
$g_J = 6/5$
$\mu = (\frac{6}{5})(\frac{15}{2}) = 9$

12e$^-$



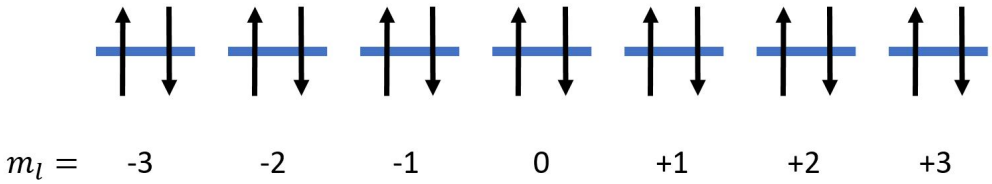
L = 3 + 2 + 1 + 0 - 1 = 5
S = 1
J = 5 + 1 = 6
Term Symbol: $^3H_6$
$g_J = 7/6$
$\mu = (\frac{7}{6})(6) = 7$

13e$^-$

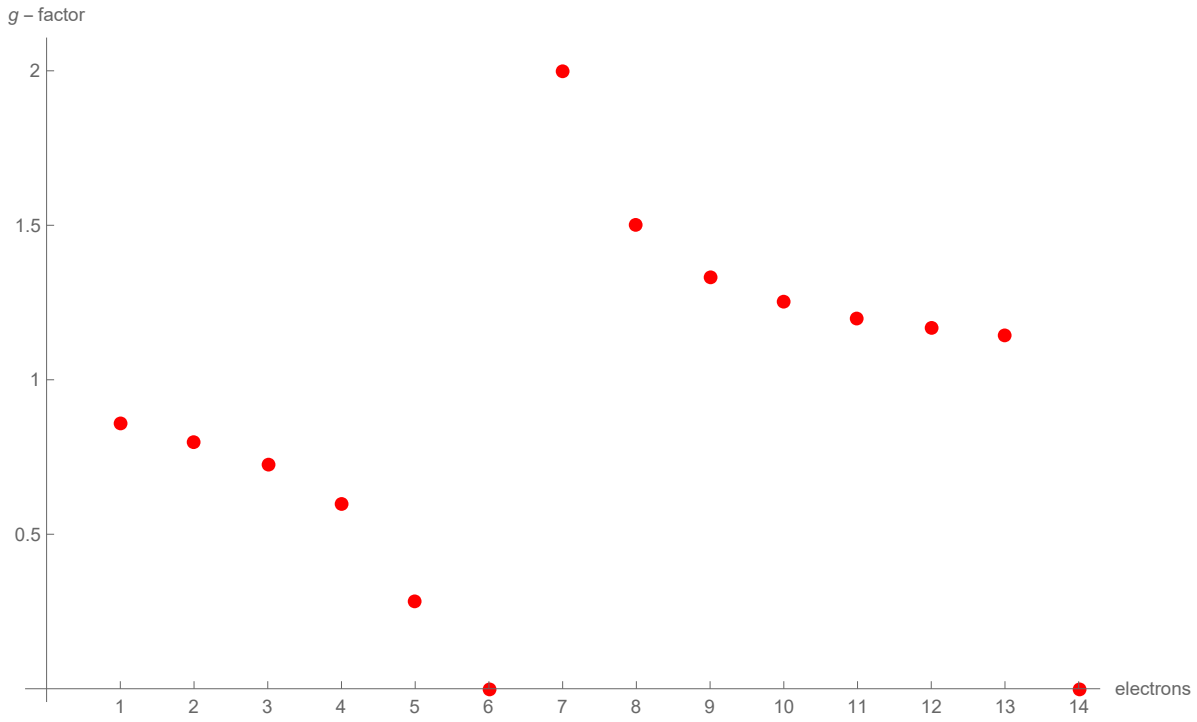


L = 3 + 2 + 1 + 0 - 1 - 2 = 3
S = 1/2
J = 3 + 1/2 = 7/2
Term Symbol: $^2F_{7/2}$
$g_J = 8/7$
$\mu = (\frac{8}{7})(\frac{7}{2}) = 4$

14e$^-$



L = 3 + 2 + 1 + 0 - 1 - 2 - 3 = 0
S = 0
J = 0
Term Symbol: $^1S_0$
$g_J = 0$
$\mu = 0$


g – factor
2
1.5
1
0.5
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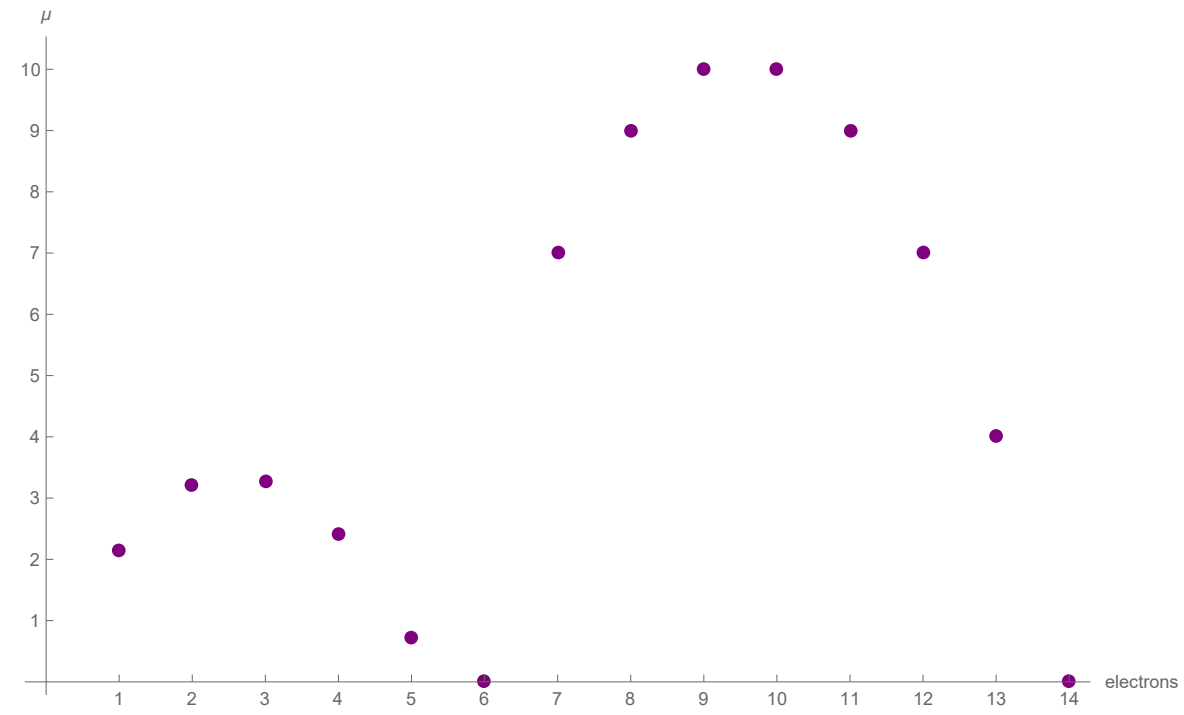
6
7
8
9
10
11
12
13
14
electrons


μ
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electrons