CHM225: PROBLEM SET #5.

1. Li: $1s^2 2s^1$

the properly anti-symmetrized wavefunction can be written in terms of a slater determinant.

$$\psi_{Li} = \frac{1}{\sqrt{3!}} \begin{vmatrix} 1s(1)\alpha(1) & 1s(2)\alpha(2) & 1s(3)\alpha(3) \\ 2s(1)\alpha(1) & 2s(2)\alpha(2) & 2s(3)\alpha(3) \\ 2s(1)\beta(1) & 2s(2)\beta(2) & 2s(3)\beta(3) \end{vmatrix}$$

Expanding along first row:

$$= \frac{1}{\sqrt{3!}} \times \Big[1s(1)\alpha(1)\big[2s(2)\alpha(2)\cdot 2s(3)\beta(3) - 2s(2)\beta(2)2s(3)\beta(3)\big] - 1s(2)\alpha(2)\big[2s(1)\alpha(1)\cdot 2s(3)\alpha(3) - 2s(1)\beta(1)\cdot 2s(3)\alpha(3)\big] + 1s(3)\alpha(3)\big[2s(1)\alpha(1)2s(2)\beta(2) - 2s(1)\beta(1) - 2s(2)\alpha(2)\big]$$

Possible Term Symbols:

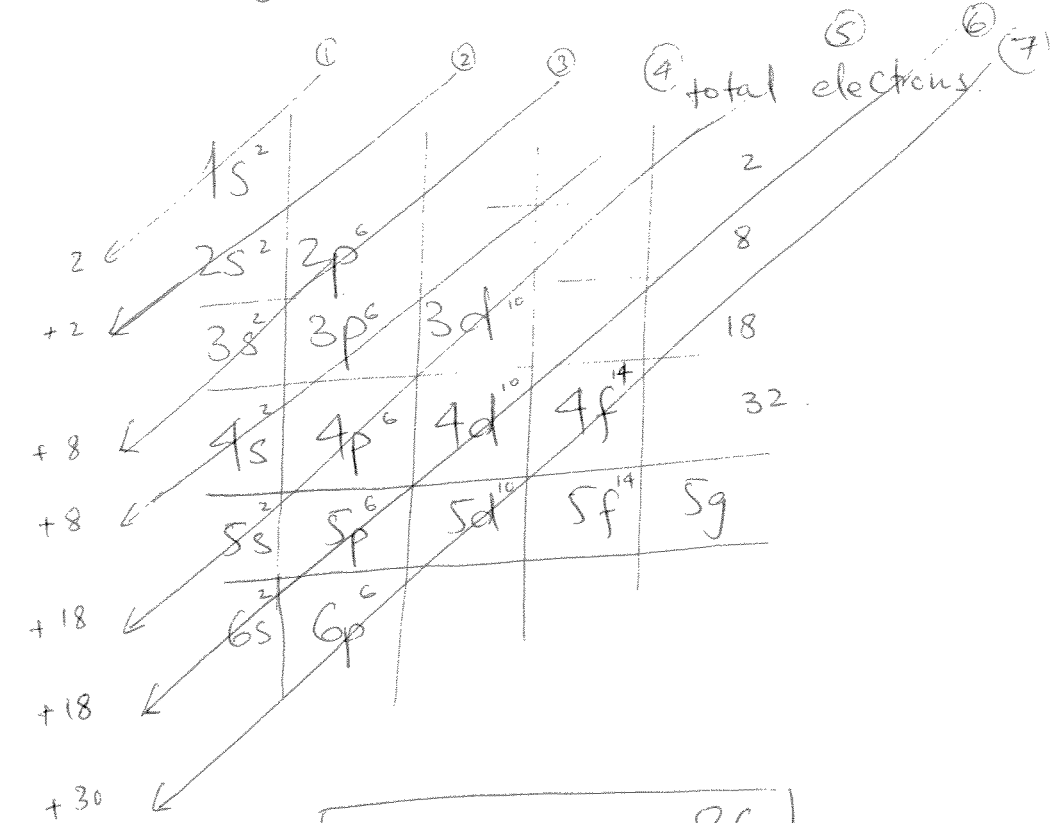
Only need to consider unfilled shell.

$2s^1$: $l = 0$; $s = 1/2$.

$2s+1 = 2$.

^2S

2. Madelung Principle (first atom with filled 6p shell).



Atomic # : 86

3. Ground State electronic configuration of:

^{35}Br: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$

^{53}I: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^5$

Q4. Term Symbols of Beryllium:

a) $1s^2 2s^2$: only closed shells

$\Rightarrow L=0, S=0$

Term Symbol: ^1S

b) $1s^2 2s^1 2p^1$: We consider only the open orbitals.

$2s^1 \quad 2p^1$

$\downarrow \quad \downarrow$

$l_1=0 \quad l_2=1$

$s_1=1/2 \quad s_2=1/2.$

recall that, L, the combined orbital angular momentum can take all values in the range.

$$|l_1 - l_2| \leq L \leq |l_1 + l_2|$$

$$|0-1| \leq L \leq |0+1|$$

$$L = 1$$

Similarly the combined spin angular momentum, S: $|s_1 - s_2| \leq S \leq |s_1 + s_2|$

$$0 \leq S \leq 1$$

$S=0$ or $S=1$.

$\Rightarrow$ Term Symbol: $^1P \quad ^3P$

$L=1$