

ADVANCED CHEMISTRY 2008

QUANTUM MECHANICS - SPRING - WEEK 1

Term symbols for the first 36 elements

H $1s^1$ $\frac{1}{1s}$ $M_L = 0 \Rightarrow L = 0$ $M_S = \pm \frac{1}{2} \Rightarrow S = \frac{1}{2}$ } $J = \frac{1}{2}$

$2S_{1/2}$

He $1s^2$ 1s completely filled orbitals $\Rightarrow L = 0$ $S = 0$ $J = 0$ $1S_0$

Li $1s^2 2s^1$ $\frac{1}{2s}$ $M_L = 0$ $M_S = \pm \frac{1}{2} \Rightarrow L = 0$ $S = \frac{1}{2} \Rightarrow J = \frac{1}{2}$

$2S_{1/2}$

Be $1s^2 2s^2$ completely filled orbitals $\Rightarrow L = 0, S = 0$ $J = 0$

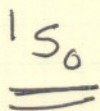
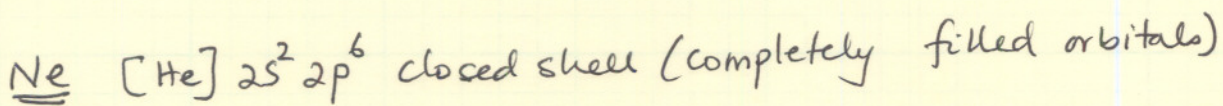
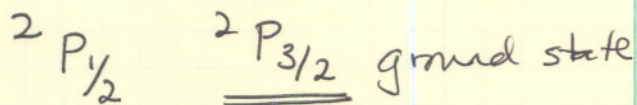
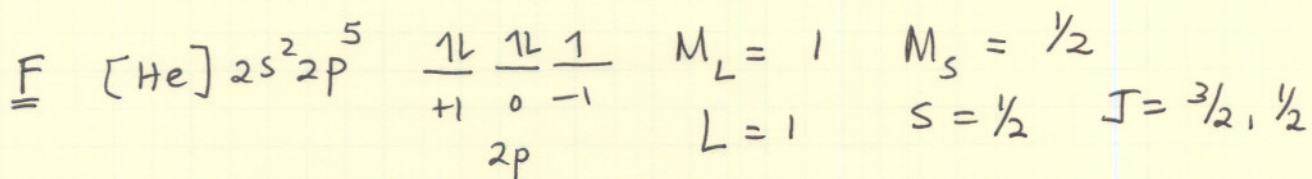
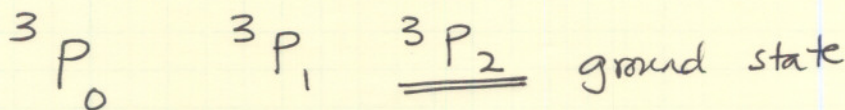
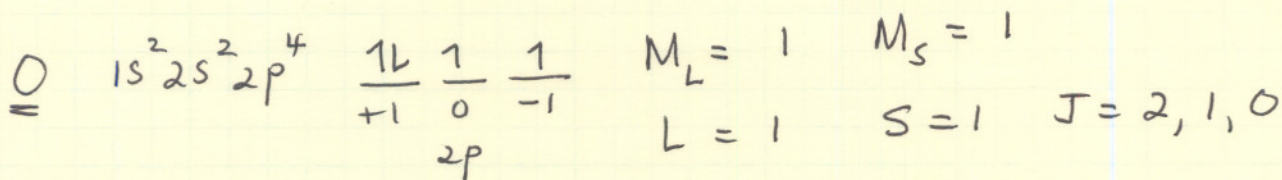
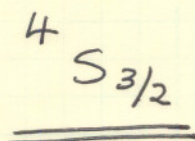
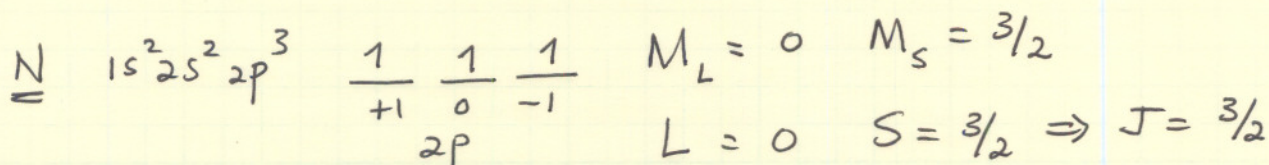
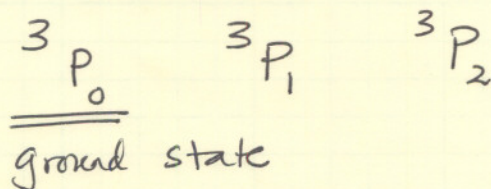
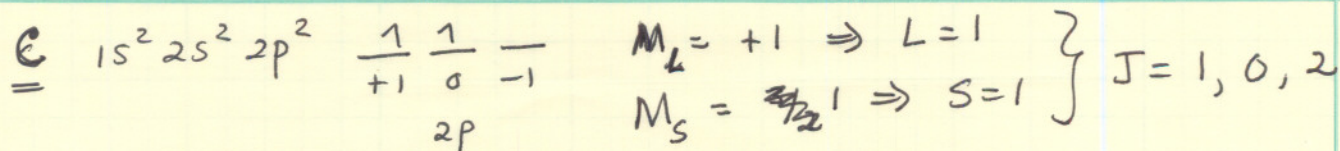
$1S_0$

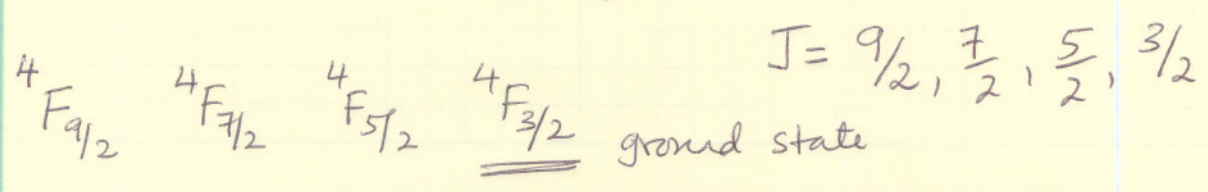
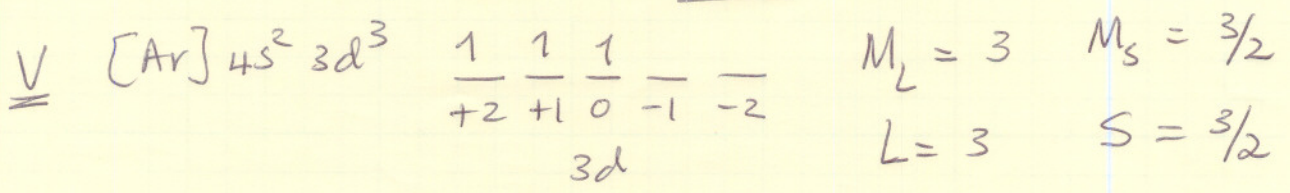
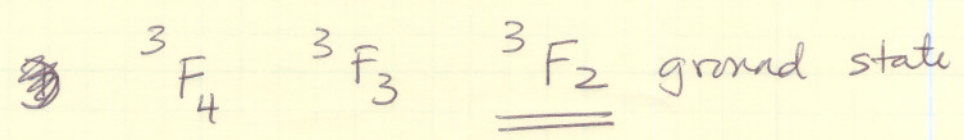
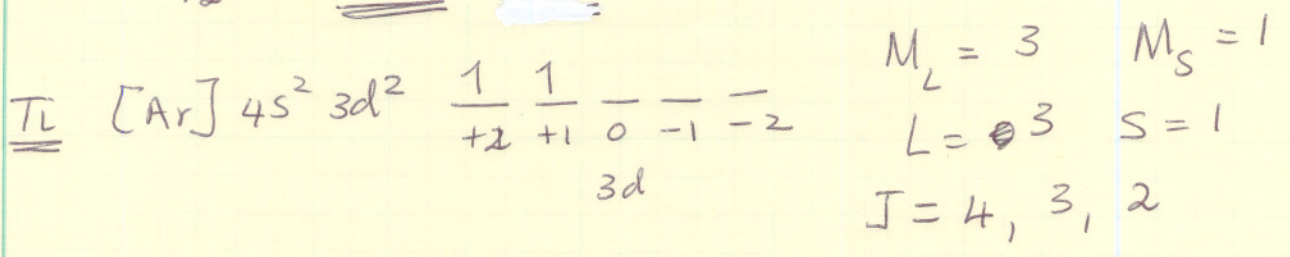
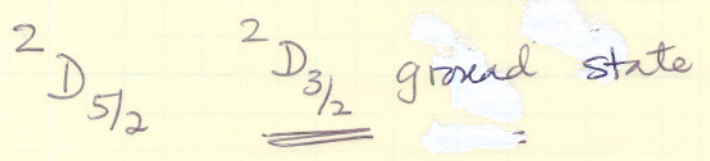
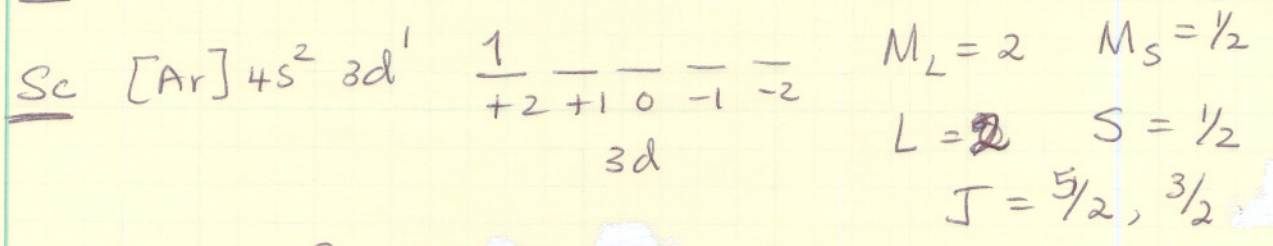
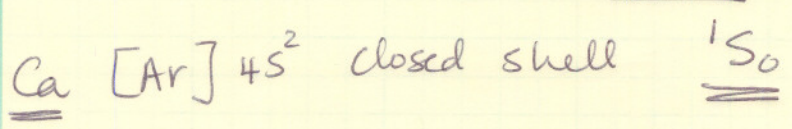
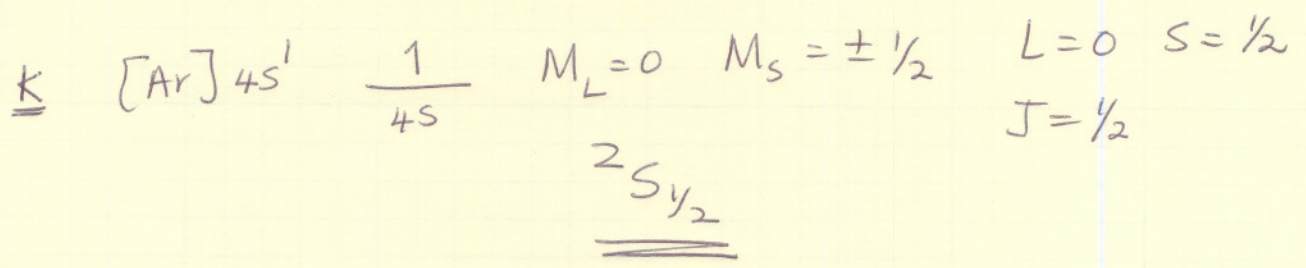
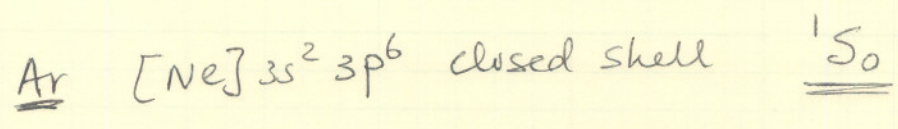
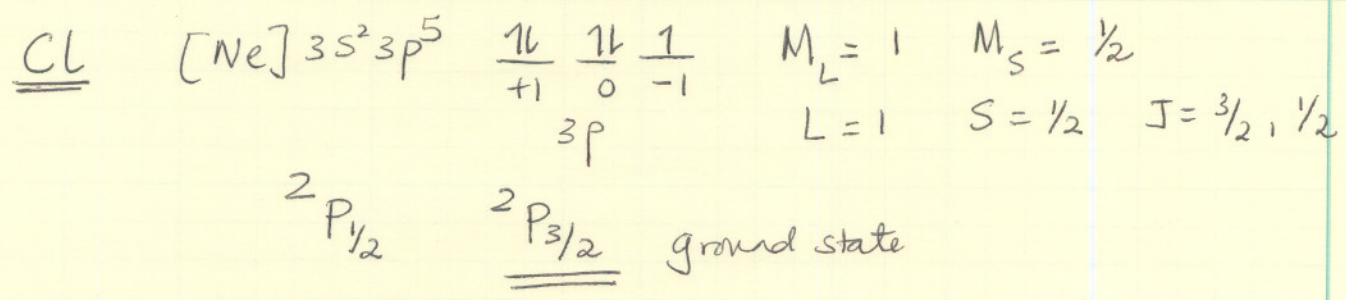
B $1s^2 2s^2 2p^1$ $\frac{1}{2p}$ $\begin{matrix} +1 & 0 & -1 \\ \hline & & \end{matrix}$ $M_L = 1$ $M_S = \pm \frac{1}{2} \Rightarrow L = 1$ $S = \frac{1}{2}$

$\Rightarrow J = \frac{1}{2}, \frac{3}{2}$

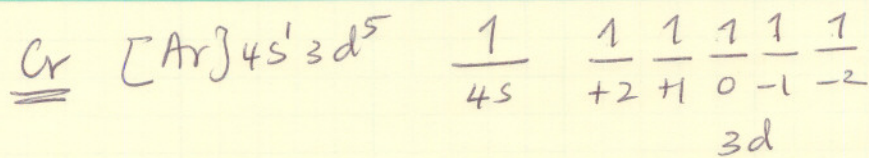
$2P_{1/2}$ and $2P_{3/2}$

ground state using Hund's rules





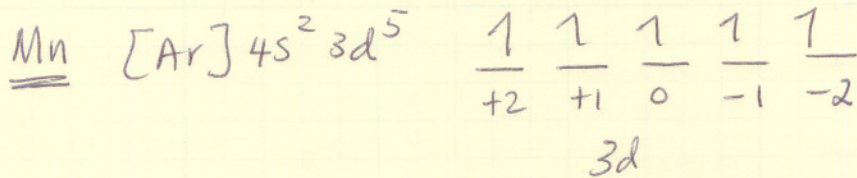
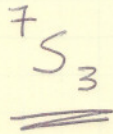
$3 + 1/2$
 $4 + 1/2$



$$M_L = 0 \quad M_S = 3$$

$$L = 0 \quad S = 3$$

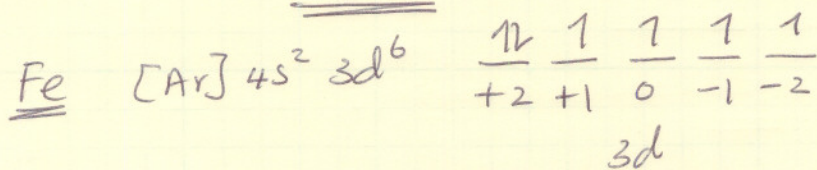
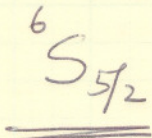
$$J = 3$$



$$M_L = 0 \quad M_S = 5/2$$

$$L = 0 \quad S = 5/2$$

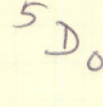
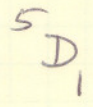
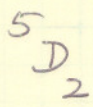
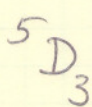
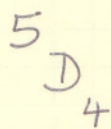
$$J = 5/2$$



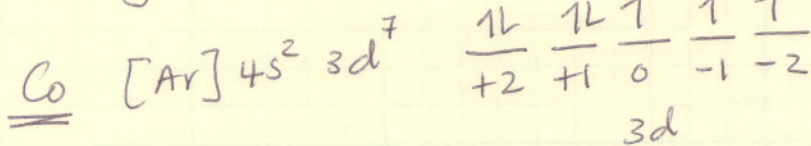
$$M_L = 2 \quad M_S = 2$$

$$L = 2 \quad S = 2$$

$$J = 4, 3, 2, 1, 0$$



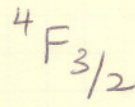
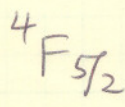
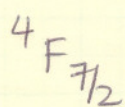
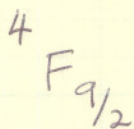
ground state



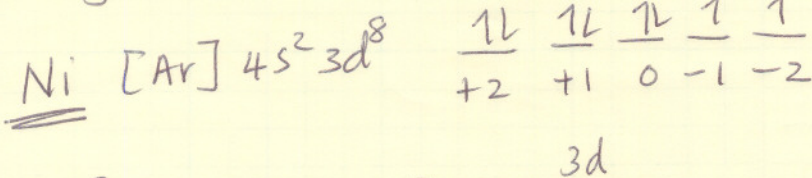
$$M_L = 3 \quad M_S = 3/2$$

$$L = 3 \quad S = 3/2$$

$$J = \frac{9}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$$



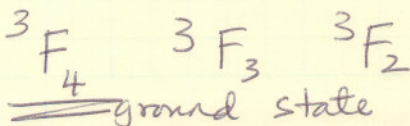
ground state

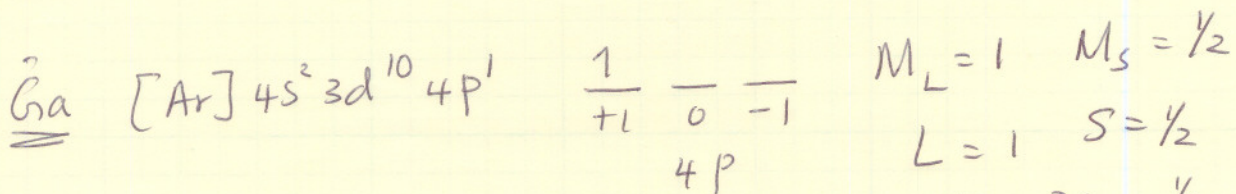
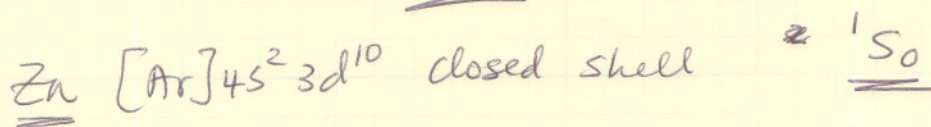
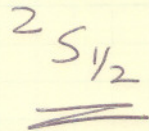
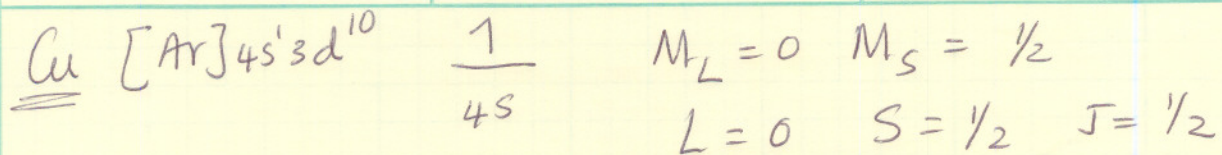


$$M_L = 3 \quad M_S = 1$$

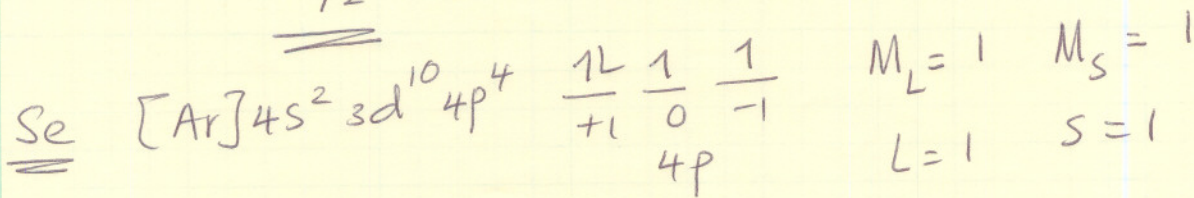
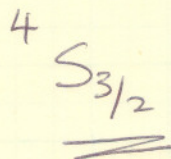
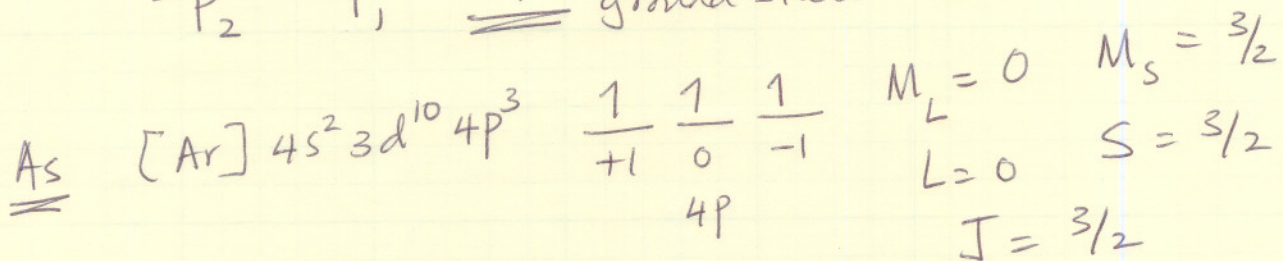
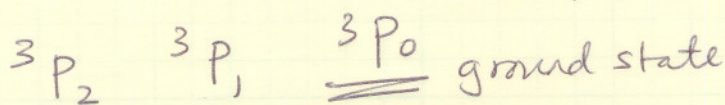
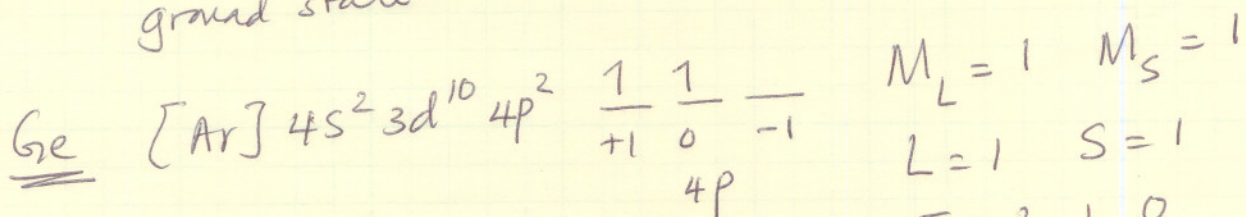
$$L = 3 \quad S = 1$$

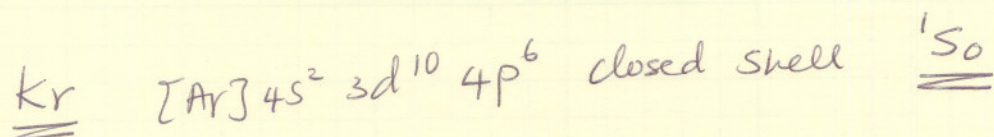
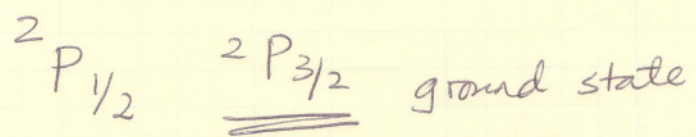
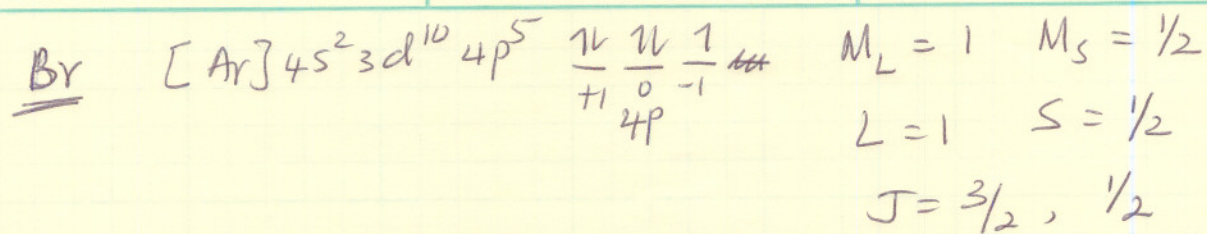
$$J = 4, 3, 2$$





ground state





Chapter 10

(29) (a) $\psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_B(1) & \psi_B(2) \end{vmatrix}$

$$\psi = \psi_A(1)\psi_B(2) - \psi_B(1)\psi_A(2)$$

If we interchange the two columns, the new wavefunction

$$\psi' = \begin{vmatrix} \psi_A(2) & \psi_A(1) \\ \psi_B(2) & \psi_B(1) \end{vmatrix} = \psi_A(2)\psi_B(1) - \psi_B(2)\psi_A(1)$$

$$= -\psi$$

∴ Interchanging the columns changes the sign of the wavefunction

Interchanging the two rows we get

$$\psi'' = \begin{vmatrix} \psi_B(1) & \psi_B(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_B(1)\psi_A(2) - \psi_A(1)\psi_B(2)$$

$$= -\psi$$

\therefore interchanging the rows changes the sign of the wavefunction.

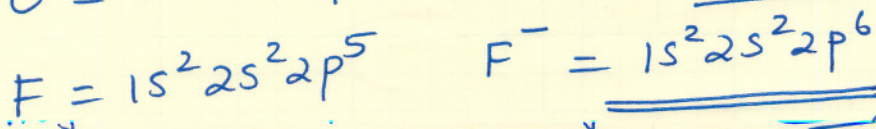
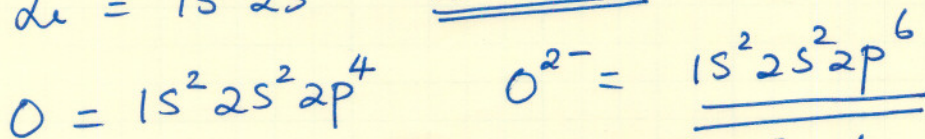
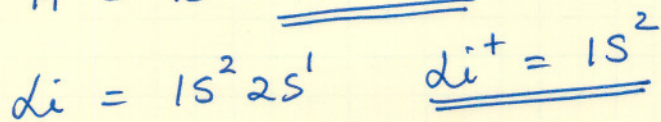
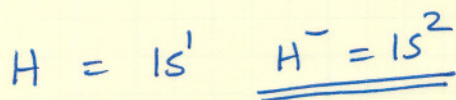
(c) If the two electrons have the same spin orbital, then $\psi_A(1) = \psi_B(1)$

$$\text{then } \psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_A(1)\psi_A(2) - \psi_A(1)\psi_A(2) = 0$$

\Rightarrow the wavefunction is zero

\Rightarrow the two electrons cannot have the same spin orbital.

(30)



(31)

1s 2e⁻

2s 2e⁻

2p 6e⁻

3s 2e⁻

3p 6e⁻

3d 10e⁻

(60)

$$\psi = \begin{vmatrix} 1s\alpha(1) & 1s\beta(1) \\ 1s\alpha(2) & 1s\beta(2) \end{vmatrix} = 1s\alpha(1)1s\beta(2) - 1s\alpha(2)1s\beta(1)$$

$$\hat{P}_{12} \psi = \begin{vmatrix} 1s\alpha(2) & 1s\beta(2) \\ 1s\alpha(1) & 1s\beta(1) \end{vmatrix} = 1s\alpha(2)1s\beta(1) - 1s\alpha(1)1s\beta(2) = -\psi$$

since $\hat{P}_{12} \psi = -\psi$, the wavefunction is antisymmetric w.r.t. interchange of electrons.

(63)

$$Sc = [Ar] 4s^2 3d^1$$

$$Sc^+ = [Ar] 4s^1 3d^1 \quad Sc^{2+} = [Ar] 3d^1$$

$$Sc^{3+} = [Ar] = 1s^2 2s^2 2p^6 3s^2 3p^6$$