

Atoms

$$\text{Helium: } H = \left\{ -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_1} \right\} \\ + \left\{ -\frac{\hbar^2}{2m} \nabla_2^2 - \frac{1}{4\pi\epsilon_0} \frac{2e^2}{r_2} \right\} \\ + \frac{1}{4\pi\epsilon_0} \frac{e^2}{|r_1 - r_2|}$$

$\psi(r_1, r_2) = \psi_{nlm}(r_1) \psi_{n'l'm'}(r_2)$ is only approximate because of the last term.

Order of filling l : smaller $l \Rightarrow$ more tightly bound \Rightarrow lower P.E. due to screening when further out. Fill small l first.

$n=1, l=0$ H, He

$n=2, l=0$ Li, Be

$n=2, l=1$ B, C, N, O, F, Ne

$n=3, l=0$ Na, Mg

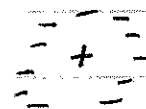
$n=3, l=1$ Al, Si, P, S, Cl, Ar

Screening so strong overlap w/ next n

$\rightarrow n=4, l=0$ K, Ca

$n=3, l=2$ Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn

$n=4, l=1$ Ga, Ge, As, Se, Br, Kr



effective Z smaller
for outer electrons

Atomic physics nomenclature:

Carbon: $(1s)^2(2s)^2(2p)^2$

$$^{2S+1}L_J$$

S = total spin

L = total orbital angular momentum

J = total angular momentum

For carbon 3P_0

$S=1$ $L=1$ $J=0$

Angular momentum:

Overall wavefunction antisymmetric upon interchanging two particles.

For two s-electrons:

$$\psi(r_1, r_2) = \underbrace{\psi_{1s}(r_1)\psi_{1s}(r_2)}_{\text{symmetric}} \underbrace{\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}_{\text{antisymmetric}}$$

→ overall antisymmetric

What about two p-electrons ($l=1$)?

orbital state

$L=2$

symmetric

$L=1$

antisymmetric

$L=0$

symmetric

spin state

$S=1$

symmetric

$S=0$

antisymmetric

} see CG coefficients

⇒ An antisymmetric wavefunction can be made from

$L=2, S=0$
 1D

$L=1, S=1$
 3P

$L=0, S=0$
 1S

(see Problem 5.13)

Hund's rule (or Hund's first rule) says
highest spin has the lowest energy:

$3p.$