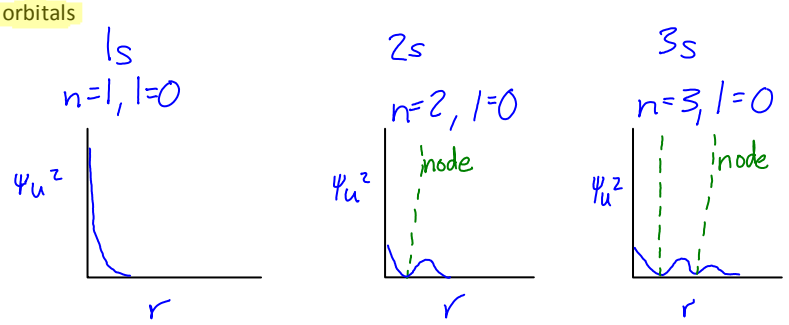
Notes 01/09

Wednesday, January 09, 2008
10:06 AM

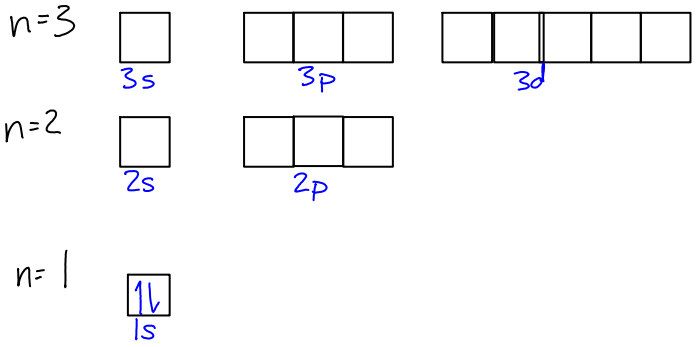
Notes 0109

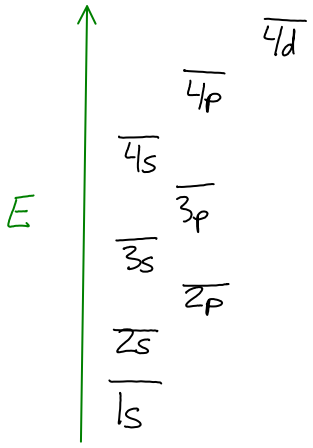
Audio recording started: 10:07 AM Wednesday, January 09, 2008

S orbitals

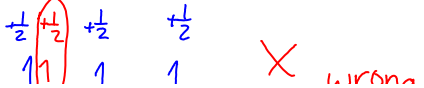


Energy Diagram





Filling electrons in energy diagrams:



$+\frac{1}{2}$ $+\frac{1}{2}$ $+\frac{1}{2}$ $+\frac{1}{2}$

↑↑ ↑ ↑ ✗ wrong

↑↓ ↑ ↑ ← lowest energy → correct

Pauli Exclusion Principle - no more than 2 in an orbital and spins must be paired.

↑↑↑ _ _ ✗ → wrong

↑ ↑ ↓ okay but not lowest energy

Hund's Rule: When more than one orbital is available for occupation at a certain energy level, electrons must occupy separate orbitals.

Examples:

- Fe $1s2s2p3s3p4s3d$ → long notation
  Fe $[Ar]4s^2 3d^6$ → short notation
  some books write $Fe[Ar]3d^6 4s^2$ → okay also

- $Fe^I = Fe^{+1}$ = lost $1e^-$ from Fe
  $Fe[Ar]4s^2 3d^6$
  $Fe^I[Ar]3d^7$

  When you ionize transition metals, generally take electrons out of s orbital and not d with 2 exceptions. This happens since 4s and 3d are very similar in energy.

- $Rh[Kr]5s^2 4d^7$
  $Rh^I[Kr]4d^8$
  $Rh^{III}[Kr]4d^6$

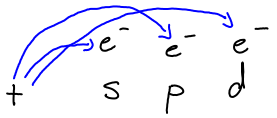
- ~~$Cr[Ar]4s^2 3d^4$~~ less favored
  $Cr[Ar]4s^1 3d^5$ lowery energy, more stable
  $Cr^{III}[Ar]3d^3$
  $Cr^I[Ar]3d^5$

  Lower energy due to the fact 4s and 3d are so close in energy and it is favorable to place electrons unpaired first.... So these exceptions are exactly 1/2 full in 4s and 3d.

- ~~$Cu[Ar]4s^2 3d^9$~~ less favored
  $Cu[Ar]4s^1 3d^{10}$ lower energy, more stable

Shielding:

Look at attraction of nucleus to electrons



$$E \propto \frac{Z_{effective}}{n^2}$$

Zeffective: effective nuclear charge
z=nuclear charge
n=principle quantum number
σ=screening or sheilding

Periodic trend:

Left to right Zeff increases
Top to bottom Zeff increases

1st row transition elements are much smaller than 2nd row transition elements. The 2nd and 3rd rows are about the same size though due to the Lanthanide contraction which is the addition of poor shielding f orbitals.

Size (radius): When add protons, radius decreases
When add electrons, radius increases

$Ti^{I} < Ti$

$Ti^{II} < Ti^{I}$

Compare size

O^{2-} F^{-} Ne Na^{+} Mg^{2+}