CHEM 362 – FALL 2020
M. Y. Darensbourg

For In-Class and PLTL Study Groups ***Week of August 24***

Worksheet II

Useful Formulas:

$E_{ion} = -Z^2/n^2$ (13.6 eV)	$E_{ion} = -Z_{eff}^2/n^2$ (13.6 eV)
$\mu(s.o.) = 2\sqrt{S\,(S+1)}$	Ground State Term Symbol: $^{(2S\ +\ 1)}L$
$S = \Sigma m_s$	$L = \Sigma m_\ell$

Slater's Rules:

1) First, write the electron configuration for the atom as follows:
(1*s*)(2*s*,2*p*)(3*s*,3*p*) (3*d*) (4*s*,4*p*) (4*d*) (4*f*) (5*s*,5*p*)

2) Any electrons to the right of the electron of interest contributes no shielding. (Approximately correct statement.)
3) All other electrons in the same group as the electron of interest shield to an extent of 0.35 nuclear charge units
4) If the electron of interest is an *s* or *p* electron: All electrons with one less value of the principal quantum number shield to an extent of 0.85 units of nuclear charge. All electrons with two less values of the principal quantum number shield to an extent of 1.00 units.

5) If the electron of interest is an *d* or *f* electron: All electrons to the left shield to an extent of 1.00 units of nuclear charge.

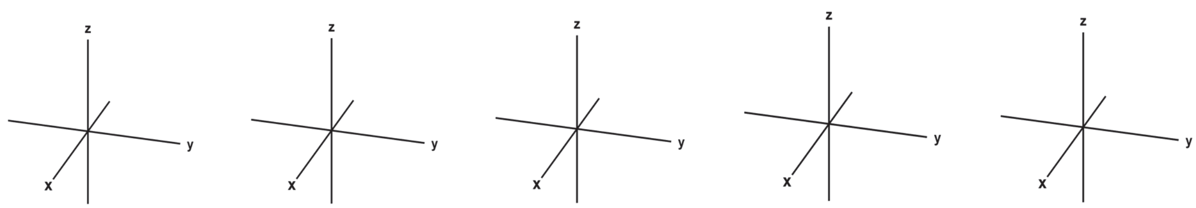
6) Sum the shielding amounts from steps 2 - 5 and subtract from the nuclear charge value to obtain the effective nuclear charge.

I. Using complete subshell notation, ($1s^22s^22p^6$, and so forth), give the electron configuration of each of the following atoms: (for example, F = $1s^2$, $2s^2$, $2p^5$)

a. N
b. Si
c. Fe
d. Te
e. V

II. On the following axes system, sketch the orbital indicated and place signs or phases or orbital lobes:

s px dxy dx2-y2 dz2



III. Using complete subshell notation ($1s^22s^22p^6$, and so forth), predict the electron configurations of the following ions. Note: Some are in unusual oxidation states!

a. N^{3-}
b. Ca^{2+}
c. S^{-}
d. Cs^{2+}
e. Cr^{2+}
f. Gd^{3+}

IV. Which of the following atoms contains only three valence electrons: Li, B, N, F, Ne? What four quantum numbers define those valence electrons?

V. Write the electron configurations for the following atoms or ions:

a. B^{3+}
b. O^{-}
c. Cl^{3+}
d. Ti

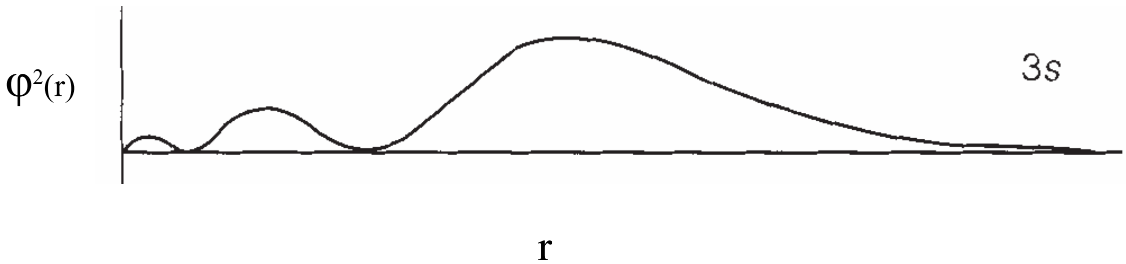
VI.

a) What are the quantum numbers (N, l, m_l, m_s) for the last electron added into the d orbitals of a Co^0 atom? (Hint: Use the box diagram approach to get your bearings.)

b) What is the relationship between radial and angular nodes? How many nodes does any orbital have?

c) How many <u>angular</u> nodes are in a 3d orbital?

d) How many <u>radial</u> nodes are found in that 3d orbital? Show this graphically by superimposing the radial distribution function of the d orbital versus r, the distance from the nucleus, over that of the 3s orbital shown below.



e) From your drawing in d), describe the difference between the contribution of a 3s electron to Slater's screening constant vs. that of a 3d electron. According to Slater, why should the experimentally observed electronic configuration of potassium, K^0, $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$, be the ground state rather than the configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1$?

f) What is the ground state term symbol for each of the configurations expressed for K^0 in e)? What is the ground state term symbol for K^+?

VII. Give ground state electronic configurations of the following, using core notation [inert gas] $ns^? np^? nd^?$. Using Slater's rules, calculate Z_{eff} on the outermost electron for each.

a. Br ____________________________ c. Ti ______________________________

b. O_____________________________ d. Mn^0 ______________________________

c. O^{2-}_____________________________ f. Sb ______________________________