Name: _____ Date: _____ CHEM 1A

Monday/Tuesday, November 18 & 19, 2019 – Quantum Chemistry & Periodic Trends (Chapter 12 Part 2)

I. **Warm-Up –** Define the words *wavefunction* and *probability density*. Also draw a Bohr model of the atom and discuss the important takeaways from the model.

Wavefunction (ψ) = A solution of the Schrödinger equation; the probability amplitude.

Probability Density (ψ^2) = A function that, when multiplied by volume of the region, gives the probability that the particle will be found in that region of space, between 0 and 1.

The Bohr model explains the Rydberg formula for spectral line emission of hydrogen.

II. **Quantum Numbers, Orbitals, & Electron Configurations**

Quantum Number	Formal Name	What it tells you	Range of Values
n	*principal quantum number*	*the size and energy of the orbital*	1 to infinity
l	*angular momentum quantum number*	*shape of the subshell*	*0 to n – 1*
m_l	*magnetic quantum number*	*orbital orientation*	*–l to +l*
m_s	*electron spin quantum number*	*Spin of the electron*	*+1/2 or –1/2*

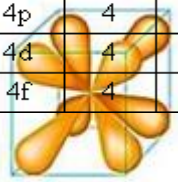
Orbitals

s orbitals ⇒ l = 0 ⇒
1 possible orientation ($m_l = 0$)

p orbitals ⇒ l = 1 ⇒ 3 possible orientations
($m_l = –1$, $m_l = 0$, $m_l = +1$)

d orbitals ⇒ l = 2 ⇒ 5 possible orientations ($m_l = –2$, $m_l = –1$, $m_l = 0$, $m_l = +1$, $m_l = +2$)

f orbitals ⇒ l = 3 ⇒ 7 possible orientations
($m_l = –3$, $m_l = –2$, $m_l = –1$, $m_l = 0$, $m_l = +1$, $m_l = +2$, $m_l = +3$)



	n	*l*	*m*	*s*
1s	1	0	0	½, - ½
2s	2	0	0	½, - ½
2p	2	1	1, 0, -1	½, - ½
3s	3	0	0	½, - ½
3p	3	1	1, 0,-1	½, - ½
3d	3	2	2, 1, 0, -1, -2	½, - ½
4s	4	0	0	½, - ½
4p	4	1	1, 0, -1	½, - ½
4d	4	2	2, 1, 0, -1, -2	½, - ½
4f	4	3	3, 2, 1, 0, -1, -2, -3	½, - ½

1. How many electrons in any one atom can have the following quantum numbers?
   a. $n = 5$ ⇒ *50*
   b. $n = 6$, $l = 0$ ⇒ *2*
   c. $n = 4$, $l = 2$ ⇒ *10*
   d. $n = 4$, $l = 3$, $m_l = -2$ ⇒ *4*
   e. $n = 2$, $l = 0$, $m_l = 0$, $m_s = -1/2$ ⇒ *1*

2. Write the ground state electron configuration to determine the number of unpaired electrons in each of the following: a. Cl b. Ni c. Cr d. Ag e. Te^{2-} f. Ba^{2+}
   Cl ⇒ $1s^2 2s^2 2p^6 3s^2 3p^5$ ⇒ 1 unpaired
   Ni ⇒ $[Ar]4s^2 3d^8$ ⇒ 2 unpaired
   Cr ⇒ $[Ar]4s^1 3d^5$ ⇒ 6 unpaired
   Ag ⇒ $[Kr]5s^1 4d^{10}$ ⇒ 1 unpaired
   Te^{2-} ⇒ $[Kr]\ 5s^2 4d^{10} 5p^6$ ⇒ 0 unpaired
   Ba^{2+} ⇒ $[Kr]\ 5s^2 4d^{10} 5p^6$ ⇒ 0 unpaired

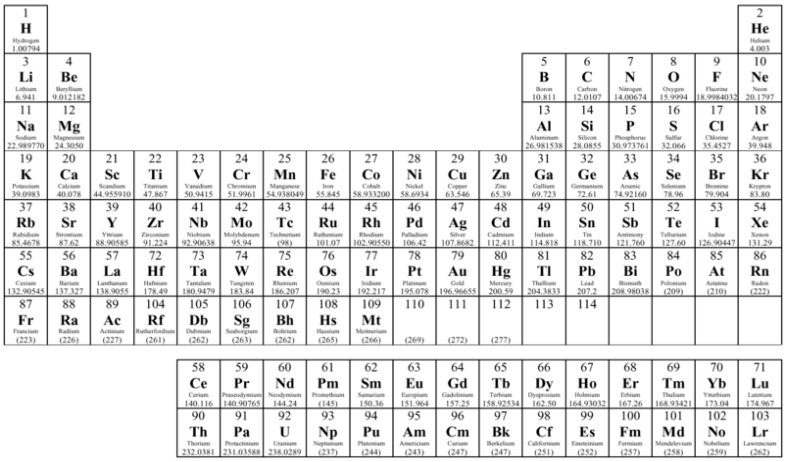
Order of Orbital Filling

Electron Configuration: A list of an atom's occupied orbitals with the number of electrons that each contains. In the **ground state** the electrons occupy atomic orbitals in such a way that the total energy of the atom is a minimum.
Pauli Exclusion Principle: No more than two electrons may occupy any given orbital. When two electrons occupy one orbital, the spins must be paired.

3. Which of the following is *not* determined by the principal quantum number, *n*, of the electron in a hydrogen atom?

a. the size of the corresponding atomic orbital(s)
b. the shape of the corresponding atomic orbital(s)
c. the energy of the electron
d. the minimum wavelength of the light needed to remove the electron from the atom.
e. All of the above are determined by *n*.

4. Determine if each of the following corresponds with an excited state or ground state electron configuration.
   a. $[Ar]4s^24p^5$ ⇒ *excited*
   b. $[Kr]6s^1$ ⇒ *excited*
   c. $[Ne]3s^23p^4$ ⇒ *ground*



III. Periodic Trends

5. Which of the following has the largest radius?
   a. Al or Si
   b. F or Cl
   c. S or S^{2-}
   d. K or K^+

6. Which of the following has the greatest ionization energy?
   a. K or Ca
   b. P or As
   c. Sr or Sr^{2+}

7. Which of the following has the most negative electron affinity?
   a. Br or Kr
   b. C or Si

The successive ionization energies for an unknown element are:

I_1 = 896 kJ/mol
I_2 = 1752 kJ/mol
I_3 = 14,807 kJ/mol
I_4 = 17,948 kJ/mol

Which family does the unknown element most likely belong? Group 2 - When you notice a jump in the order of magnitude going from 10^3 to 10^4 this implies that all of the valence electrons have been removed and the 10^4 magnitude would be referring to the core – the first and second ionization energies are within reason however the third ionization energy is much higher – therefore there must have been only 2 electrons in the valences shell.

Effective Nuclear Charge (Zeff): The net nuclear charge after considering the shielding caused by other electrons in the atom. Increases as you move right.

Atomic Radii: Half the distance between the centers of neighboring atoms in a solid of a homonuclear molecule. Increases left and down.

First Ionization Energy: The minimum energy required to remove the first electron from the ground state of a gaseous atom, molecule, or ion. X(g) -> X+(g) +e-. Increases right and up.

Electron Affinity: (Eea) The energy change associated with the addition of an electron to a gas-phase atom. X(g) + e- ◊ X- (g) Increases left and down. (Energy release is negative, F has the lowest EA)