

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	<i>principal quantum number</i>	<i>the size and energy of the orbital</i>	1 to infinity
l	<i>angular momentum quantum number</i>	<i>shape of the subshell</i>	0 to $n - 1$
m_l	<i>magnetic quantum number</i>	<i>orbital orientation</i>	$-l$ to $+l$
m_s	<i>electron spin quantum number</i>	<i>Spin of the electron</i>	$+1/2$ or $-1/2$

Orbitals

s orbitals $\Rightarrow l = 0 \Rightarrow$

1 possible orientation ($m_l = 0$)



p orbitals $\Rightarrow l = 1 \Rightarrow 3$ possible orientations

($m_l = -1, m_l = 0, m_l = +1$)



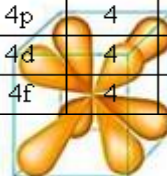
d orbitals $\Rightarrow l = 2 \Rightarrow 5$ possible orientations (m_l

$= -2, m_l = -1, m_l = 0, m_l = +1, m_l = +2$)



f orbitals $\Rightarrow l = 3 \Rightarrow 7$ 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_l	m_s
1s	1	0	0	$\frac{1}{2}, -\frac{1}{2}$
2s	2	0	0	$\frac{1}{2}, -\frac{1}{2}$
2p	2	1	1, 0, -1	$\frac{1}{2}, -\frac{1}{2}$
3s	3	0	0	$\frac{1}{2}, -\frac{1}{2}$
3p	3	1	1, 0, -1	$\frac{1}{2}, -\frac{1}{2}$
3d	3	2	2, 1, 0, -1, -2	$\frac{1}{2}, -\frac{1}{2}$
4s	4	0	0	$\frac{1}{2}, -\frac{1}{2}$
4p	4	1	1, 0, -1	$\frac{1}{2}, -\frac{1}{2}$
4d	4	2	2, 1, 0, -1, -2	$\frac{1}{2}, -\frac{1}{2}$
4f	4	3	3, 2, 1, 0, -1, -2, -3	$\frac{1}{2}, -\frac{1}{2}$

1. How many electrons in any one atom can have the following quantum numbers?

- $n = 5 \Rightarrow 50$
- $n = 6, l = 0 \Rightarrow 2$
- $n = 4, l = 2 \Rightarrow 10$
- $n = 4, l = 3, m_l = -2 \Rightarrow 4$
- $n = 2, l = 0, m_l = 0, m_s = -1/2 \Rightarrow 1$

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 $\Rightarrow 1s^2 2s^2 2p^6 3s^2 3p^5 \Rightarrow 1$ unpaired

Ni $\Rightarrow [\text{Ar}] 4s^2 3d^8 \Rightarrow 2$ unpaired

Cr $\Rightarrow [\text{Ar}] 4s^1 3d^5 \Rightarrow 6$ unpaired

Ag $\Rightarrow [\text{Kr}] 5s^1 4d^{10} \Rightarrow 1$ unpaired

$\text{Te}^{2-} \Rightarrow [\text{Kr}] 5s^2 4d^{10} 5p^6 \Rightarrow 0$ unpaired

$\text{Ba}^{2+} \Rightarrow [\text{Kr}] 5s^2 4d^{10} 5p^6 \Rightarrow 0$ 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?
- the size of the corresponding atomic orbital(s)
 - the shape of the corresponding atomic orbital(s)
 - the energy of the electron
 - the minimum wavelength of the light needed to remove the electron from the atom.
 - 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.
- $[\text{Ar}]4s^24p^5 \Rightarrow \text{excited}$
 - $[\text{Kr}]6s^1 \Rightarrow \text{excited}$
 - $[\text{Ne}]3s^23p^4 \Rightarrow \text{ground}$

III. Periodic Trends

5. Which of the following has the largest radius?
- Al** or Si
 - F or **Cl**
 - S or **S²⁻**
 - K** or K⁺

1 H Hydrogen 1.00794																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012182											5 B Boron 10.811	6 C Carbon 12.01107	7 N Nitrogen 14.00644	8 O Oxygen 15.9994	9 F Fluorine 18.9984032	10 Ne Neon 20.1797
11 Na Sodium 22.989770	12 Mg Magnesium 24.3050											13 Al Aluminum 26.981538	14 Si Silicon 28.0855	15 P Phosphorus 30.973761	16 S Sulfur 32.066	17 Cl Chlorine 35.4527	18 Ar Argon 39.948
19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.955910	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9961	25 Mn Manganese 54.938049	26 Fe Iron 55.845	27 Co Cobalt 58.933200	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.61	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.80
37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.94	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.90550	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.90447	54 Xe Xenon 131.29
55 Cs Cesium 132.90545	56 Ba Barium 137.327	57 La Lanthanum 138.9055	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9479	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.078	79 Au Gold 196.96655	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.98038	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
87 Fr Francium (223)	88 Ra Radium (226)	89 Ac Actinium (227)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (263)	107 Bh Bohrium (262)	108 Hs Hassium (265)	109 Mt Meitnerium (266)	110 Ds Darmstadtium (269)	111 Rg Roentgenium (272)	112 Cn Copernicium (277)						
58 Ce Cerium 140.116	59 Pr Praseodymium 140.90765	60 Nd Neodymium 144.24	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.92534	66 Dy Dysprosium 162.50	67 Ho Holmium 164.93032	68 Er Erbium 167.26	69 Tm Thulium 168.93482	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967				
90 Th Thorium 232.0381	91 Pa Protactinium 231.03688	92 U Uranium 238.02891	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)	103 Lr Lawrencium (262)				

6. Which of the following has the greatest ionization energy?
- K or **Ca**
 - P** or As
 - Sr or **Sr²⁺**
7. Which of the following has the most negative electron affinity?
- Br** or Kr
 - C** or Si

The successive ionization energies for an unknown element are:

$$I_1 = 896 \text{ kJ/mol}$$

$$I_2 = 1752 \text{ kJ/mol}$$

$$I_3 = 14,807 \text{ kJ/mol}$$

$$I_4 = 17,948 \text{ kJ/mol}$$

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 (Z_{eff}): 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. $X(g) \rightarrow X^+(g) + e^-$. Increases right and up.

Electron Affinity: (E_{ea}) The energy change associated with the addition of an electron to a gas-phase atom. $X(g) + e^- \rightarrow X^-(g)$ Increases left and down. (Energy release is negative, F has the lowest EA)