- 1. Electronic configurations:
  - H: 1s<sup>1</sup> Li: 1s<sup>2</sup>2s<sup>1</sup> C: 1s<sup>2</sup>2s<sup>2</sup>2p<sup>2</sup> Ne: 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup> Na: 1s<sup>2</sup>2s<sup>2</sup>2p<sup>6</sup>3s<sup>1</sup>

Greater ionization potential? The ionization potential is the amount of energy needed to remove the outermost electron. **F has a greater ionization potential than Li**, and this can be defended by several concepts from this course.

- a) The graph of ionization potential vs. z shows a general trend of increasing ionization potential from left to right across a period.
- b) If you calculated  $z_{eff}$  from the equation  $z_{eff} = z$ -(e's in inner shells)-0.9(e's in same shell, inner subshell)-0.8(e's in same shell) the  $z_{eff}$  for F is greater than that for Li. Since  $z_{eff} \propto I.P$ .
- c) Even without calculating the z<sub>eff</sub>, you could explain that, although F does have more electrons to shield it from the nucleus, this does not counteract the effect of the greater number of protons in the nucleus, so F's electrons are more tightly held by the larger nucleus.

2. Because we are talking about ejecting electrons, we need to consider the work function equation:

$$E = hv - \Phi$$

Since we have two sets of data, we can set up two equations and solve for the two unknowns.

$$\begin{array}{l} 4*10^{20} \ I = h*(2*10^{10} \ Au^{-1}) \ \text{-} \ \Phi \\ 12*10^{20} \ I = h*(3*10^{10} \ Au^{-1}) \ \text{-} \ \Phi \end{array}$$

Eq. 1 can be rearranged to:	$\Phi = (2^*10^{10} \text{ Au}^{-1})\text{h} - 4^*10^{20} \text{ I}$
And plugged into eq. 2:	$12*10^{20}$ I = h*(3*10 <sup>10</sup> Au <sup>-1</sup> ) - (2*10 <sup>10</sup> Au <sup>-1</sup> )h - 4*10 <sup>20</sup> I
And then solved for h:	$h = 8*10^{10}$ I-Au

Since h and  $\Phi$  are constants, it doesn't matter which data set you plug back into to find h to get the work function:  $\Phi=1.2*10^{21}$  I

So, the results are  $h = 8 \times 10^{10}$  I-Au and  $F = 1.2 \times 10^{21}$  I

(By the way, you were stranded in Hawaii – all the words were from a Hawaiian web dictionary)

3. Remember:

# angular nodes = quantum number "l" (where l=0 is s, l=1 is p, l=2 is d etc) # radial nodes = n-l-1, where n is the principle quantum number # total nodes = n-1

So, by figuring out the nodes correctly, you can get the type of orbital.

The first wavefunction corresponds to a 2p?. There are zero radial nodes (r=0 does not count as a node) and 1 angular plane (between zero and 180, there is only one point that is equal to zero for  $\cos\theta$ ). So, l=1 (p) and n-1-1=0, so n=2. To sketch it you have to look at the graph of the angular part:



For the second wavefunction, there are **no radial nodes** (r=0 doesn't count and  $e^{-r/ao}$  never reaches zero) and there are **two angular nodal planes**. So, *l*=2 (d) and n-2-1=0, so n=3. This is a **3d orbital** and the sketch should look something like this:



(Actually, this is the "doughnut around a P orbital" or the " $d_z^2$ " orbital on page 318 in your book, but we accepted the above "sketch" as accurate enough. You didn't have to be an artist!)

4. This is just like the homework problem we did for hexatriene. There are four electrons that we are going to assign to the particle in a box model. All four electrons in the conjugated Pi system are free to go back and forth along the length of the molecule. So, the wavefunction of each electron extends over the length of the molecule (between L=0 and L=5.78 A), but does not exist outside of these limits – just like a particle in a box. The particle in a box model has defined energy levels:

$$E_n = \frac{n^2 \hbar^2 \boldsymbol{p}^2}{2mL^2}$$

Where  $n = energy \ level$ ,  $h = Planck's \ constant$   $m = mass \ of \ one \ electron \ and \ L = length \ of \ the \ box.$ 

To figure out the energy of the highest occupied level, you need to decide which energy levels to put the electrons into. According to the Aufbau principle for particle in a box, only 2 electrons can go into each energy level, and a level that is lower in energy will fill up before the next level begins to fill. Therefore, two electrons go into the first level and 2 into the second. So the highest occupied is n=2 and the lowest unnoccupied is n=3. **E2** = **7.15E-19 J E3** = **1.61E-18 J** AE = 8.05E + 10 J = hc/2

 $\Delta E = 8.95E-19 \text{ J} = hc/\lambda$  $\mathbf{l} = 223nm$ 

	Valid	Invalid	Bonding	Antibond	Singlet	Triplet
А	Х			X		Х
В	Х		X		Х	
С		X				
D		X				
Е		X				
F	Х			Х		Х

5. The table should look like this for the given wavefunctions

Electrons must have an overall antisymmetric wavefunction. The bonding/antibonding designation comes from the symmetry of the spatial part, and the singlet triplet comes from the spin part.

- A. Anti spatial\*sym spin, therefore antisymmetric overall, allowed. Because the spatial is antisymmetric (minus sign) it is antibonding, and because the spin is symmetric it is one of the triplet states.
- B. Sym spatial\*anti spin, antisymmetric overall allowed. Because the spatial is symmetric (plus sign) it is bonding, and because the spin is antisymmetric, it is the singlet state.
- C. Sym spatial\*sym spin symmetric overall, not allowed.
- D. Anti spatial\*anti spin symmetric overall, not allowed.
- E. Sym spatial\*sym spin symmetric overall, not allowed.
- F. Anti spatial\*sym spin antisymmetric overall, allowed. Because the spatial is antisymmetric (minus sign) it is antibonding, and because the spin is symmetric, it is one of the triplet states.