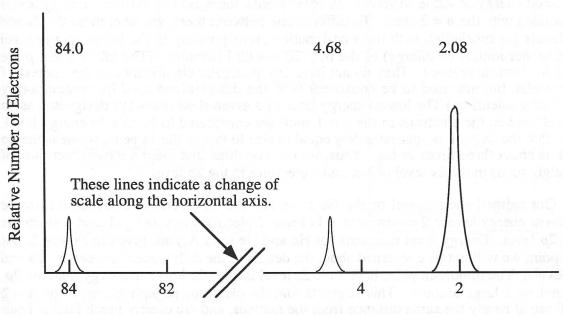
# ChemActivity 8

# The Shell Model (III) (How Many Peaks Are There in a Photoelectron Spectrum?)

#### Information

Figure 1. Simulated photoelectron spectrum of neon.



Ionization Energy (MJ/mole)

### **Critical Thinking Questions**

Is the experimental photoelectron spectrum for Ne shown in Figure 1 consistent with our model of the structure of atoms? In what ways (if any) was our prediction correct? In what ways was it not correct?

#### Model 1: The Neon Atom Revisited.

Contrary to our predictions, there are three peaks in the spectrum, not two! It appears that we must now modify our model to remain consistent with these new experimental results. We note that there is a peak at 2.08 MJ/mole (as expected) and one at a much higher energy—in this case, 84.0 MJ/mole. We can safely assume that this higher energy peak corresponds to the electrons in the n = 1 shell, and that the electrons in that shell have an energy of -84.0 MJ/mole. Thus, the other two peaks must both arise from electrons in the n = 2 shell. This suggests that there are electrons with two different energies in the n = 2 shell, some with an energy of -4.68 MJ/mole, and others with the expected energy of -2.08 MJ/mole. In other words, there are two different energy levels associated with the n = 2 shell. To differentiate between them, we label them the 2s and 2p levels (or subshells), with the s designation corresponding to the lower energy level (and higher ionization energy) of the two (IE = 4.68 MJ/mole). (The labels s and p are used for historic reasons. They do not have any particular significance in the context of our model, but are used to be consistent with the designations used by contemporary practicing scientists.) The lowest energy level of a given shell is always designated as an s level, and so the electrons in the n = 1 shell are considered to be in a 1s energy level. Note that the 2s peak is approximately equal in size to that of the 1s peak, whereas the 2p peak is about three times as big. Thus, we can conclude that there are two electrons (of the eight total) in the 2s level of Ne, and 6 electrons in the 2p level.

Our refined shell model of the Ne atom has the 10 electrons distributed in three different energy levels: 2 electrons in a 1s level, 2 electrons in a 2s level, and 6 electrons in a 2p level. Energy level diagrams for He and Ne (and Ar) are given in Figure 2. At this point we will not be concerned about the details of the differences between the 2s and 2p levels. The important point is that the 2s level is slightly lower in energy than the 2p, but not by a large amount. This suggests that the electrons in both levels of the n=2 shell are at nearly the same distance from the nucleus, and are clearly much farther from the nucleus than the electrons in the n=1 shell. Also, we have found that there appears to be a limit of 2 on the number of electrons that can be placed in an s subshell.

Figure 2. Energy level diagrams for helium, neon, and argon.

Helium
$$1s \stackrel{\bullet \bullet}{=} -2.37$$

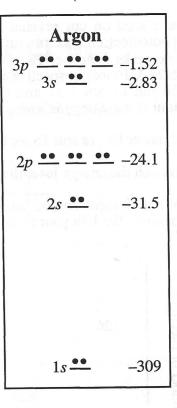
$$2p \stackrel{\bullet \bullet}{=} \stackrel{\bullet \bullet}{=} \stackrel{\bullet \bullet}{=} -2.08$$

$$-4.68$$

$$1s \stackrel{\bullet \bullet}{=} -84.0$$

The energy levels of the electrons (MJ/mole) are the negative of the ionization energies.

Energy levels are not to scale.

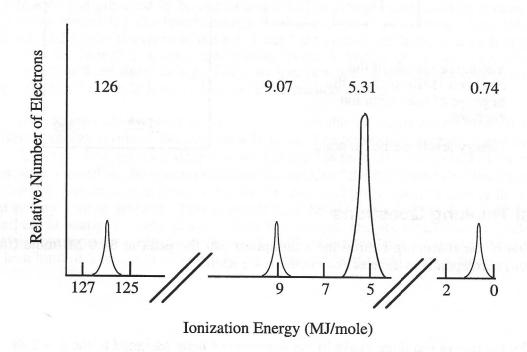


## **Critical Thinking Questions**

- 2. What is the reasoning behind the assumption that the peak at 84.0 MJ/mole (for neon) corresponds to the electrons in the n = 1 shell?
- 3. Why are two of the three peaks in the spectrum of neon assigned to the n = 2 shell, rather than to the n = 1 shell?
- 4. Why is it not important to place numbers along the y axis of photoelectron spectra?
- 5. Based on the energy level diagram in Figure 2, sketch a photoelectron spectrum for Ar. Make sure to indicate the relative intensities and positions of all peaks.

#### **Exercises**

- 1. a) Based on our revised shell model, how many peaks would be expected in a photoelectron spectrum of lithium? b) What would you expect the relative sizes of the peaks to be? c) The *ls* ionization energies for H, He, and Li are 1.31, 2.37, and 6.26 MJ/mole, respectively. Explain this trend. d) The first ionization energies for H and Li are 1.31 and 0.52 MJ/mole, respectively. Explain why the Li first ionization energy is lower.
- 2. Answer Ex. 1a and 1b for beryllium and for carbon.
- 3. Sketch the energy level diagram (as in Figure 2) for Be and for C.
- 4. What element do you think would give rise to the photoelectron spectrum shown below? Explain your reasoning.



#### **Problems**

- 1. Indicate whether each of the following statements is true or false and explain your reasoning:
  - a) The photoelectron spectrum of Mg<sup>2+</sup> is expected to be identical to the photoelectron spectrum of Ne.
  - b) The photoelectron spectrum of <sup>35</sup>Cl is identical to the photoelectron spectrum of <sup>37</sup>Cl.
- 2. The energy required to remove a 1s electron from F is 67.2 MJ/mole. The energy required to remove a 1s electron from Cl is: a) 54 MJ/mole; b) 67.2 MJ/mole; c) 273 MJ/mole; d) a 1s electron cannot be removed from Cl. Explain.