Building a Simple Model of the Atom Key

Bohr's model of the atom assumes that an electron in an atom can have only certain specified energies and that an atom absorbs or emits a photon when an electron changes its energy level. Coulomb's law suggests that each energy level is associated with a spherical orbit, or shell, at a finite distance, *d*, from the nucleus and that the electron's movement is confined to this orbit.

One weakness to Bohr's model, as currently constructed, is that it isn't clear how it extends to atoms with multiple electrons. For example, an atom of Li has three electrons, but Bohr's model doesn't indicate where these electrons normally are found. Can all three electrons reside in the shell closest to the nucleus? Is each electron in a separate shell? Or, is there some other arrangement of electrons?

We can use ionization energies to expand upon Bohr's model. Atoms with several electrons will have an ionization energy for each electron. The smallest ionization, which is for the most easily removed electron, is called the first ionization energy, or IE_1.

The first ionization energy for a H atom is 1310 kJ/mol. Assuming that both electrons in a He atom are in the same shell and at the same distance from the nucleus as in a H atom, predict the value of IE_1 for a He atom. Hint: your answer shouldn't be 1310 kJ/mol! Repeat for the Li atom. Explain your reasoning.

For He the nucleus has a charge of +2, which is twice that for the H atom. Coulomb's law, therefore, suggests that the ionization energy for helium should be twice that for the H atom, or 2620 kJ/mole. Lithium, with a +3 nucleus, should have an ionization energy of 3930 kJ/mole.

Now, find the experimental values for the first ionization energies for He and Li using the table on page 78 of your textbook. Is your prediction for He close to its experimental value? For now, assume that a value within a few hundred kJ/mol is reasonably close. Repeat for Li.

The experimental value for He is 2372 kJ/mole, which is reasonably close. The value for Li, however, is but 520 kJ/mole, which is much smaller than predicted.

Clearly the first ionization energy for Li is inconsistent with a model in which all three of its electrons are in the same orbit or shell. Assuming that Coulomb's law is still valid, what must be true about at least one of the electrons in a Li atom? Explain your reasoning.

From Coulomb's law, the only explanation is that the electron must be further from the nucleus since we know that the electron's potential energy is inversely proportional to distance.

One modification to Bohr's model is to assume that there is a limit to the number of electrons that can occupy any given energy level or shell. Look at Figure 3.7 on page 79 of your text, which shows the first ionization energies for the first 20 elements. There is a great deal of information in this figure. How many energy levels, or shells, are represented in this figure? Explain your reasoning?

There appear to be four shells because we see three places where there is a big decrease in ionization energy; from He $\rightarrow$ Li, from Ne $\rightarrow$ Na, and from Ar $\rightarrow$ K.

Let's identify the shells by number using the terminology n = 1 for the first shell, n = 2 for the second shell, and so on. How many electrons are in each of these shells for the first 18 elements? Hint – the total number of electrons must add up to 18.

n =	*number of electrons*
1	*2*
2	*8*
3	*8*

Is there a similarity between this shell model of the atom and the structure of the periodic table? If so, what is the similarity?

Yes. The number of elements in each of the first three rows (periods) of the periodic table equals the number of electrons in the first three shells.

Although your prediction for helium's first ionization energy is close to the experimental value, it is not exactly the same. Examine the difference between your predicted value and the experimental value. Which value is larger? Using Coulomb's law, provide a plausible explanation for this difference.

Our prediction of 2620 kJ/mol is larger than the experimental value of 2372 kJ/mol. We have already accounted for the effect of the helium atom having a +2 charge on the nucleus. The only other variable to consider is distance. Given our model, we must conclude, therefore, that the electrons in a helium atom are somewhat further away from the nucleus than in a hydrogen atom .

One final question. The difference between the experimental value for lithium's first ionization energy and your predicted value cannot be explained only by the electron's greater distance from the nucleus. Given Coulomb's law, what conclusion does this force upon you?

The only other variable is the charge on the nucleus. Although the charge on the nucleus of a lithium atom is +3, we must conclude that for some reason the electron does not "experience" this charge. Evidently, it "experiences" a charge that is significantly less than +3. Obviously there is a weakness in our model.