

## ChemActivity 4

# The Shell Model (I)

(How Are Electrons Arranged?)

Electrons in atoms are attracted to the nucleus by a Coulombic force. Thus, energy must be supplied (by some means) if the electron is to be pulled away from the nucleus, thereby creating a positively charged species, or **cation**, and a free electron. For real atoms, the **ionization energy** (IE) of an element is the minimum energy required to remove an electron from a gaseous atom of that element.

Ionization energies are usually obtained experimentally. One method of measuring ionization energies is the electron impact method. Atoms are bombarded with fast-moving electrons. If these electrons have sufficient energy, they will, on colliding with an atom, eject one of the atom's electrons. The ionization energy described above (often called the *first ionization energy*) corresponds to the smallest amount of energy that a bombarding electron needs to be able to knock off one of the atom's electrons.

### Model 1: First Ionization Energy (IE<sub>1</sub>).



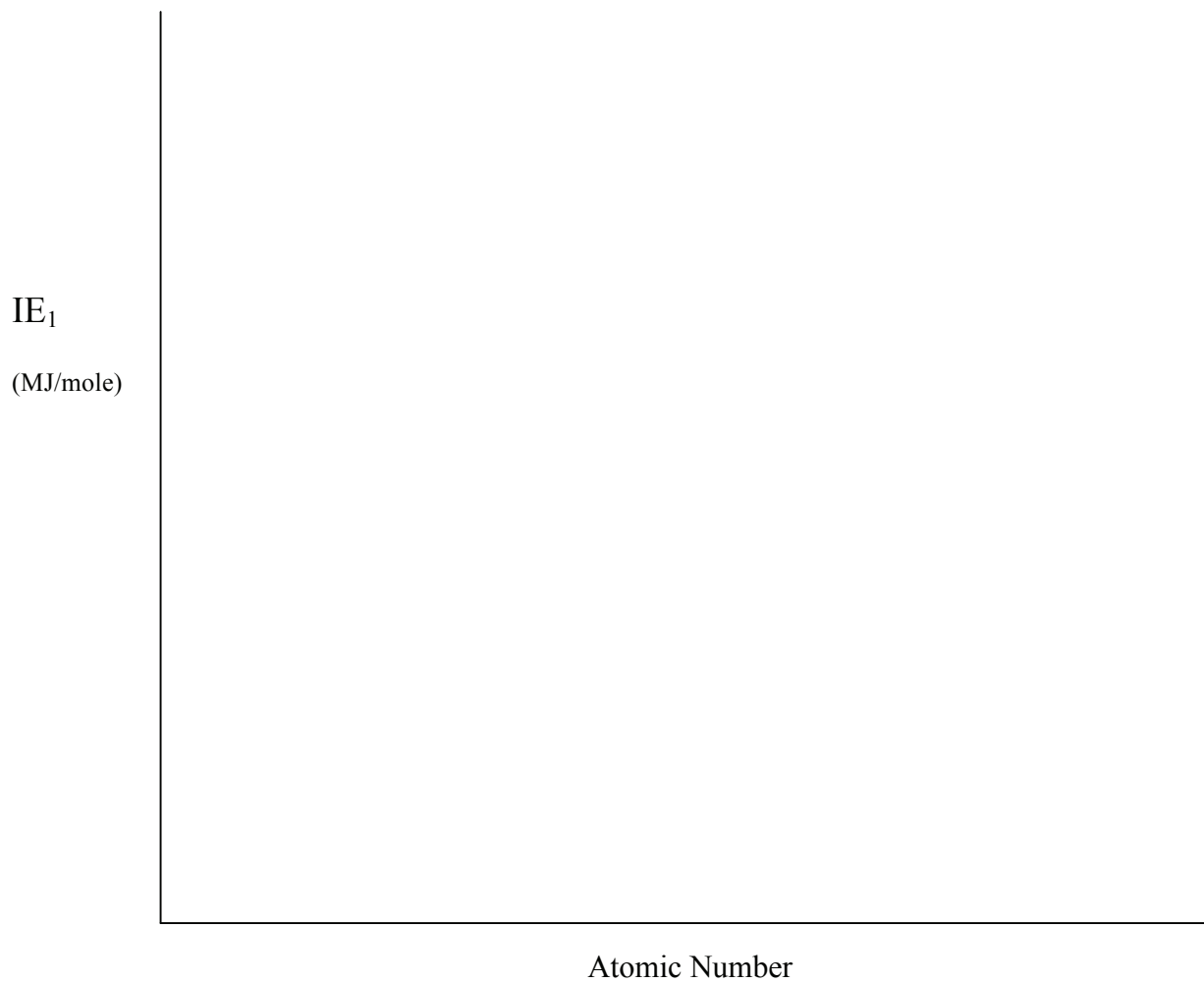
For a H atom, IE =  $2.178 \times 10^{-18}$  J.

The first ionization energy, IE<sub>1</sub>, for a single atom is a very small number of joules. For reasons of convenience, chemists have chosen to report the ionization energies of elements in terms of the minimum energy necessary to remove a single electron from each of a mole of atoms of a given element. This results in ionization energies for the elements that are in the range of MJ/mole. (Note that 1 MJ = 10<sup>6</sup> J.)

### Critical Thinking Questions

1. How much total energy would it take to remove the electrons from a mole of H atoms? Write this energy in MJ/mole.
2. For atoms with many electrons, not all electrons are at the same distance from the nucleus. In this case, which electron would have the lowest ionization energy: the electron that is closest to the nucleus or the electron that is farthest from the nucleus? Explain.

3. Predict the relationship between  $IE_1$  and atomic number by making a rough graph of  $IE_1$  vs. atomic number. DO NOT PROCEED TO THE NEXT PAGE UNTIL YOU HAVE COMPLETED THIS GRAPH.



## Information

Based on our previous examination of ionization energies, it is expected that the ionization energy of an atom would increase as the nuclear charge,  $Z$ , increases. In addition, the ionization energy of an atom should decrease if the electron being removed is moved farther from the nucleus (that is, if  $d$  increases).

Table 1 below presents the experimentally measured ionization energies of the first 20 elements. We will examine these results and attempt to propose a model for the structure of atoms based on these data.

**Table 1. First ionization energies of the first 20 elements.**

$Z$		$IE_1$ (MJ/mole)	$Z$		$IE_1$ (MJ/mole)
1	H	1.31	11	Na	0.50
2	He	2.37	12	Mg	0.74
3	Li	0.52	13	Al	0.58
4	Be	0.90	14	Si	0.79
5	B	0.80	15	P	1.01
6	C	1.09	16	S	1.00
7	N	1.40	17	Cl	1.25
8	O	1.31	18	Ar	1.52
9	F	1.68	19	K	0.42
10	Ne	2.08	20	Ca	0.59

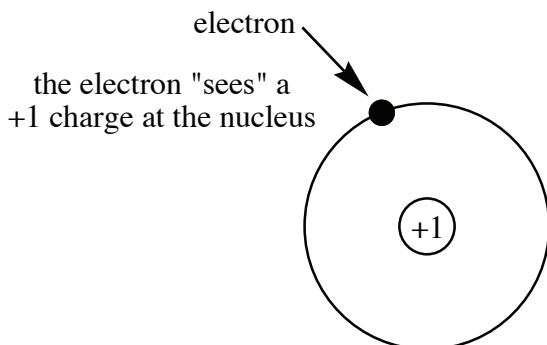
## Critical Thinking Questions

4. Compare your answer to CTQ 3 to the data in Table 1. Comment on any similarities and differences.
  
5. Using grammatically correct English sentences:
  - a) provide a possible explanation for why  $IE_1$  for He is greater than  $IE_1$  for H.
  
  - b) provide a possible explanation for why  $IE_1$  for Li is less than  $IE_1$  for He.

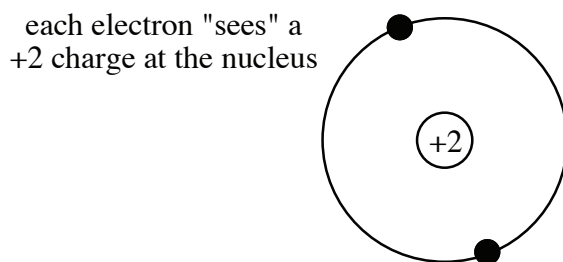
## Model 2: Simple Model Diagrams for Hydrogen and Helium Atoms.

One simple model of the hydrogen atom pictures the H atom as a nucleus of charge +1 surrounded by an electron at some distance, as shown in Figure 1.

**Figure 1. Model diagram of a hydrogen atom.**



**Figure 2. Model diagram of a helium atom.**



Examining the data in Table 1, we note that the ionization energy of He ( $Z=2$ ) is larger than that of H ( $Z=1$ ) by approximately a factor of 2. This is consistent with the two electrons in the He atom at a distance (from the nucleus) approximately the same as that in H.

### Critical Thinking Question

- The value of the ionization energy of He given in Table 1 is described as being consistent with two electrons in a "shell" approximately the same distance from the nucleus as the one electron in H. Use the Coulombic Potential Energy equation,  $V = \frac{kq_1q_2}{d}$  to explain how this conclusion can be reached. Hint: recall the relationship between  $V$  and  $IE_1$ .

## Information

Because the He nucleus has a charge of +2, we would expect that the ionization energy to remove an electron from (approximately) the same distance as in a H atom would be (approximately) twice that of the H atom. That is what we observe. We can say that there are two electrons in a **shell** around the He nucleus. Although we will present figures in which the shells appear to be circular (mostly because it is difficult to present three-dimensional representations on paper), we recognize that the model we develop is qualitatively consistent with spherical shells. Thus, within our *Shell Model*, He consists of a nucleus surrounded by 2 electrons in a single shell.

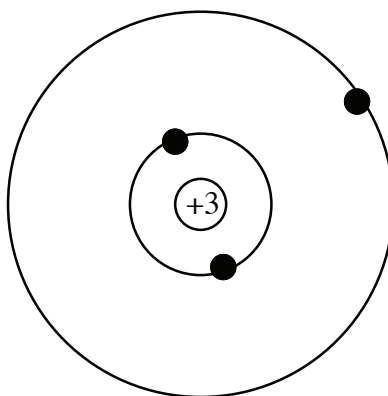
## Critical Thinking Questions

7. Recall that the IE of H is 1.31 MJ/mole. If all three electrons in Li were in the first shell at a distance equal to that of hydrogen, which of the following values would be the better estimate of the  $IE_1$  of Li: 3.6 MJ/mole or 0.6 MJ/mole? Explain.
8. A student proposes a model for the Li atom in which all three electrons are in the first shell at a distance approximately the same as in H. Why is this model not consistent with the  $IE_1$  for Li in Table 1?
9. Another student proposes a model for the Li atom in which two electrons are in the first shell (as in He) and the third electron is much farther from the Li nucleus. Explain why this model is consistent with the  $IE_1$  for Li in Table 1.

### Model 3: The Shell Model for Lithium.

For Li, there is a change in the trend of the ionization energy. The ionization energy of a Li atom is *less* than that of He. In fact, it is significantly *smaller* than that of the H atom! This is not consistent with a model of placing a third electron in the first shell, for doing so would result in an ionization energy which is larger than that of He. In order for Li to have a lower ionization energy than H, either the nuclear charge  $Z$  must be lower than that of H, or the distance of the easiest-to-remove electron from the nucleus must be greater than in H (and He), or both. We know that the nuclear charge is *not* lower than that of H; thus, the electron being removed must be farther from the nucleus than the first shell. Although the data we have does not require us to choose the following model, let us assume that the structure of Li involves two electrons in a first shell (as in He) with the third electron placed in a second shell, with a significantly larger radius, as shown in Figure 3.

**Figure 3.** Diagram of a lithium atom using the shell model.



### Critical Thinking Question

- Is the amount of energy required to remove one of the electrons from the first shell of Li greater than, less than, or equal to the  $IE_1$  for Li? Explain your reasoning.

## Exercises

1. A scientist proposes a model for the helium atom in which both electrons are in a "shell" which is half the distance from the nucleus as the electron in a hydrogen atom. Is this model consistent with the data in Table 1? Explain your reasoning. (Hint: according to the Coulombic Potential Energy equation, how much more strongly does a nuclear charge of +2, as in He, hold an electron than a nuclear charge of +1, as in H? According to the Coulombic Potential Energy equation, how much more strongly does a nuclear charge hold an electron if it is at  $d/2$ , rather than  $d$ ?)
2. Propose an alternative model for the lithium atom which is consistent with the data in Table 1.

## Problem

1. a) Write the three Coulombic Potential Energy terms for the helium atom model in Figure 2. Assume that the distance between each electron and the nucleus is  $d$  and that the distance between the two electrons is  $2d$ .  
  
b) Based on your answer to part a) explain why the IE of He is slightly less than twice the IE of H even though both atoms are about the same size.