First Ionization Energies for H → Ar Key

Element	IE_1 (kJ/mol)	Element	IE_1 (kJ/mol)	Element	IE_1 (kJ/mol)
H	1310	N	1400	Al	580
He	2370	O	1310	Si	790
Li	520	F	1680	P	1010
Be	900	Ne	2080	S	1000
B	800	Na	500	Cl	1250
C	1090	Mg	740	Ar	1520

1. One modification to the simple shell model is to limit the number of electrons that can occupy any energy level, or shell. Examine the first ionization energies for the elements H through Ar. How many energy levels, or shells, are suggested by this data? Explain how the data supports your answer?

   This data suggests that there are three shells because we see two places where there is a significant decrease in ionization energy; from He → Li and from Ne → Na.

2. Let's identify the shells as follows: $n = 1$ for the first shell, $n = 2$ for the second shell, and so on. For the first 18 elements, how many shells are there and how many electrons are in each shell? Explain how the data supports your answer?

   For n = 1 there are two electrons, for n = 2 there are eight electrons, and for n = 3 there are eight electrons, giving a total of 18 electrons.

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

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

4. Helium's first ionization energy is almost, but not quite twice that of hydrogen's, which suggests that both electrons are in the same shell. Using Coulomb's law, suggest one or more reasons why the first ionization energy for He is slightly smaller than expected?

   The only possible explanations are that the distance between the electrons and the nucleus is about 10% greater in He than in H, or that the electrons in He see a charge on the nucleus that is about 10% less than expected, or some combination of the two. We know that IE_1 is proportional to $-(q_+)(q_-)/d$, so we can solve for relative changes in any of these terms by assuming that the proportionality constant is 1 and is the same for all elements (note: the proportionality constant simply converts a unit of charge squared per distance into a unit of force; it is the same for all elements).

   if we solve $1310 = -(+1)(-1)/d$ for d, we get 0.00076 as the radius for hydrogen

   if we solve $2370 = -(+2)(-1)/d$ for d, we get 0.00084 as the radius for helium, an increase of 10%

   if we solve $2370 = -(q)(-1)/0.00076$ for q, we get 1.8 as the charge on the nucleus, a decrease of 10%

5. Lithium's first ionization energy is much smaller than that for hydrogen, which we can explain by assuming that two electrons are in an $n = 1$ shell and one electron is an $n = 2$ shell. Which shell gives rise to IE_1 for lithium?

   The first ionization energy is for the electron in the n = 2 shell because it is furthest from the nucleus; we call electrons in the outermost shell valence electrons and we identify all other electrons as core electrons.

6. We call the electrons in lithium's $n = 1$ shell core electrons and those in its $n = 2$ shell valence electrons. Considering that the core electrons are closer to the nucleus than the valence electrons, and considering Coulomb's law, what might you conclude about the values of q_+ and q_- for an electron in lithium's $n = 2$ shell?

   We expect that q_- is independent of shell, as it is the charge of the electron; thus, its value is –1. The meaning of q_+ is more nuanced, as the core electrons in the n = 1 shell reside between the nucleus and the valence electron in the n = 2 shell; our best approximation is to assume that q_+ is Z – number of core electrons, which gives q_+ as +1 for lithium; we call this the effective nuclear charge, Z_{eff}.

7. Do the relative values of IE_1 make sense for elements in the same column?

   Yes. The shell model suggests that each row in the periodic table is a new shell that is further from the nucleus; thus, we expect IE_1 to decrease down a column as Z_{eff} remains constant but distance increases.

8. What other interesting trends do you see in the first ionization energies? What questions do they raise for you?

   Within a shell we expect ionization energies to increase with Z; however, we see a decrease from Be → B, from N → O, from Mg → Al, and from P → S. Any explanation must reside in Coulomb's law in terms of q_+ and/or d. Clearly our model needs additional work.