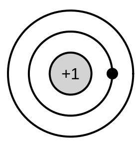
Key for First Ionization Energy Worksheet

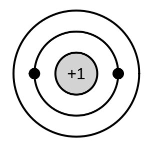
The first ionization energy, IE_1, for an element is the energy needed to remove whatever electron is easiest to remove. We can write this as a reaction

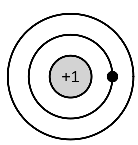
$$A \longrightarrow \mathrm{A}^{+} + \mathrm{e}^{-}$$

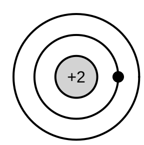
where A is the element. We know from Coulomb's Law and the mathematical derivation of the simple shell model that an electron's ionization energy is proportional to the ratio of the charge on the nucleus, Z, and the distance between the electron and the nucleus, which is the radius of the shell in which the electron resides, R; thus, $IE \propto Z/r$.

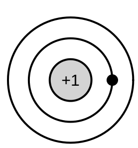
Each of the following pairs of diagrams show representations of hypothetical elements, where the central shaded circle represents a nucleus with the specified charge, the outer circles are shells, and the solid dots are electrons. For each pair, use the relationship $IE \propto Z/r$ and decide which of the two elements has the larger first ionization energy, or if their first ionization energies are identical. Explain your decisions.

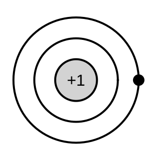












- For the first pair, we expect that IE_1 is the same for both as each has the same Z and the same r.
- For the second pair, the one on the right has the larger IE_1 as both have the same r, but the one on the right has the larger Z and ionization energies are directly proportional to Z.
- For the third pair, the one on the left has the larger IE_1 as both have the same Z, but the one on the left has the smaller r and ionization energies are inversely proportional to r.

The first ionization energies for H, He, and Li are 1310, 2370, and 520 kJ/mol, respectively. This data for He is reasonably consistent with that for H if both have as single shell; however, the data for Li suggests that the three electrons do not occupy a single shell. Explain why the data is consistent with these two interpretations.

- The Z for He is 2× that for H, so we can reasonably expect that IE_1 for He is approximately 2× that for H, even if they have slightly different values for r.
- The Z for Li is 3× that for H, so we can reasonably expect that if all of its electrons are in the same shell, that it would have an IE_1 that is more than 3000 kJ/mol. Given the surprisingly small value for IE_1, at least one of its electrons must be at a significantly greater distance from the nucleus, which suggests a second shell.

Table 1: First ionization energies for H $\longrightarrow$ Ar

element	Z	IE_1 (kJ/mol)	element	Z	IE_1 (kJ/mol)	element	Z	IE_1 (kJ/mol)
H	1	1310	N	7	1400	Al	13	580
He	2	2370	O	8	1310	Si	14	790
Li	3	520	F	9	1680	P	15	1010
Be	4	900	Ne	10	2080	S	16	1000
B	5	800	Na	11	500	Cl	17	1250
C	6	1090	Mg	12	740	Ar	18	1520

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

- The data suggests there are three shells because there are two places where we find a significant decrease in ionization energy; from He $\longrightarrow$ Li and from Ne $\longrightarrow$ Na.

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 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.

Is there a similarity between this simple shell 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: 2, 8, and 8.

Helium's first ionization energy is almost, but not quite twice that of hydrogen's, which suggests both of its electrons are in the same shell. Using Coulomb's law, suggest one or more reasons why IE_1 for He is slightly smaller than expected?

- Given that Coulomb's law depends on just the charge on the nucleus, Z, and the radius of the shell, r, the only possible explanations are that the distance between the electrons and the nucleus is a little bit bigger for He than for H, or that the electrons in He "see" a charge on the nucleus that is less than expected, or some combination of the two. What it means to "see" a smaller Z is not clear.

Lithium's first ionization energy is much smaller than that for hydrogen, which we can explain if 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.

Compare the values of IE_1 for elements in the second row to the elements directly below them in the third row? What pattern do you see? What does this imply about the relative importance of Z and r as we move from the second row to the third row?

- Within a group, the value of IE_1 for an element in the third row is smaller than the element in the second row. Given that Z increases down a group, this works to increase the ionization energy, the relative effect of r must be much more important.

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

- Within a shell we expect ionization energies to increase with Z; however, we see a decrease from Be $\longrightarrow$ B, from N $\longrightarrow$ O, from Mg $\longrightarrow$ Al, and from P $\longrightarrow$ S. Clearly our model needs additional work.