Name: ____ Period:______

5 ChemActivity 5

The Shell Model (II)

Information: The Shell Model for Li.

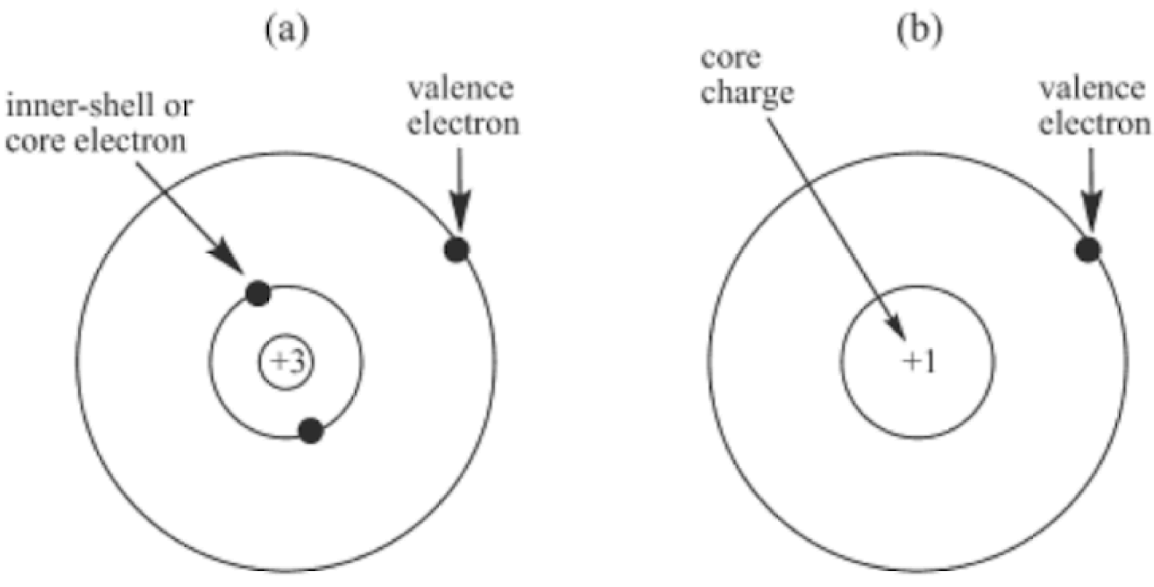
For lithium, there is a change in the trend of the ionization energy compared to hydrogen and helium. The ionization energy of a lithium atom is *less* than that of helium. In fact, it is significantly *smaller* than that of the hydrogen atom! This is not consistent with a model of placing a third electron in the first shell, for doing so would result in an ionization energy that is larger than that of helium. In order for lithium to have a lower ionization energy than hydrogen, either the nuclear charge Z for lithium must be lower than that of hydrogen, or the distance of the easiest-to-remove electron from the nucleus must be greater than in hydrogen (and helium), or both. We know that the nuclear charge of lithium is *not* lower than that of hydrogen; thus, the easiest-to-remove electron must be farther from the nucleus than the first shell in hydrogen. Although the data we have does not require us to choose the following model, let us assume that the structure of lithium involves two electrons in a first shell (as in helium) with the third electron placed in a second shell, with a significantly larger radius, as shown in Figure 1a.

Model 1: Valence Electrons, Inner-Shell Electrons, Core Charge, and Electron-Electron Repulsion

The electrons in the outermost shell of an atom are referred to as **valence** electrons. Electrons in any other shells closer to the nucleus are called **inner-shell** electrons (or core electrons). Thus, lithium has one valence electron and two inner-shell electrons. Hydrogen has one valence electron and no inner-shell electrons.

The nucleus plus the inner shells of electrons constitute the **core** of the atom, and the net overall charge on the core is called the **core charge**. We can represent the lithium atom in terms of core charge as shown in Figure 1b.

Figure 1. **Diagram of a lithium atom using (a) the shell model and (b) the core charge concept.**



Notice that within the shell model of the lithium atom, shown in Figure 1a, the valence electron is farther from the nucleus than the two inner-shell electrons. Although we have ignored it up to this point, we should remember that all of the electrons repel each other because they are negatively charged. Of particular interest is the repulsion of the valence electrons by the two inner-shell electrons. This dramatically decreases the overall force of attraction pulling the valence electron towards the nucleus.

Thus, the outer-shell valence electrons experience the charge of the core rather than the full charge of the nucleus. The core electrons that surround the nucleus are said to *shield* the nucleus from the valence electrons. In fact, because the valence electrons are all negatively charged, they repel each other also. Thus the net resulting

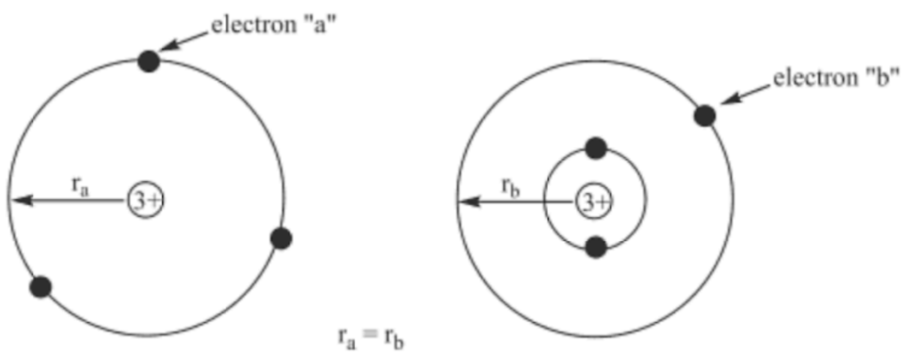
Name: ______________________________ Period:_______

charge acting on a valence electron to attract it toward the nucleus differs from the core charge. This overall resulting charge acting on a valence shell electron is known as the **effective nuclear charge**, and it is generally less than the core charge. Since there is no simple way to obtain values for the effective nuclear charge, we will use the core charge as a basis for our qualitative explanations. Core charge is only an approximation for effective nuclear charge, but it is adequate for our purposes.

1. Complete the following table:

Atom	Total number of electrons	Number of valence shell electrons	Number of inner shell electrons	Core charge
H				
He				
Li				

2. Two possible models for arrangement of electrons in lithium are shown below:

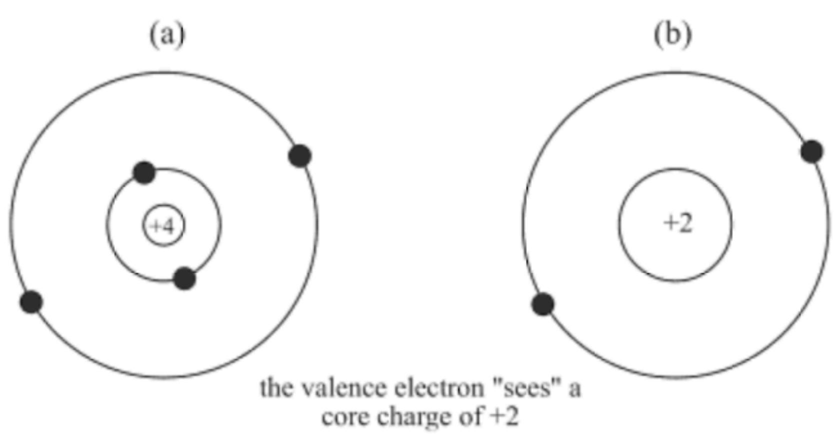


Explain why the IE_1 of electron "b" would be less than the IE_1 of electron "a".

Model 2: The Beryllium Atom.

The next element, beryllium, has an ionization energy which is larger than that for lithium. This larger IE is consistent with the fourth electron in beryllium being added to the second shell. Thus, beryllium has 2 valence electrons and a core charge of +2. Two representations of the beryllium atom are given in Figure 2.

Figure 2: Diagram of beryllium atom using (a) the shell model and (b) the core charge concept.



Name: ____ Period:_______

3. For beryllium:
   a. Why is the nuclear charge of beryllium "+4"?

   b. How many inner-shell electrons does beryllium have?

   c. How many valence electrons does beryllium have?

   d. Show how the core charge for beryllium was calculated.

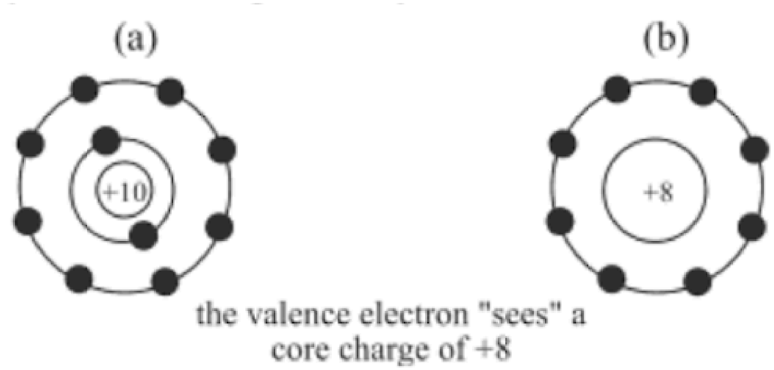
   e. Based on your answers to questions 1, 3c and 3d, what is the relationship between the number of valence electrons and the core charge of a neutral atom?

4. Assuming that the valence shells of lithium and beryllium are at approximately the same distance from their nuclei, explain how the core charges of lithium and beryllium are consistent with the IE_1 values for lithium (0.52MJ/mole) and beryllium (0.90MJ/mole).

Model 3: The Neon Atom

Although there are some slight variations, the data in Table 1 of CA4 show that in general there is an increase in IE as the atomic number further increases up to Z=10 (neon). This general trend is qualitatively consistent with a corresponding increase in core charge. There is no large drop in ionization energy to a value less than that of hydrogen, as we observed in going from helium to lithium, to indicate that a third shell is needed. This pattern in IE suggests that as we move from beryllium up to neon, the number of electrons in the second shell increases.

Figure 3: Diagram of a neon atom using (a) the shell model and (b) the core charge concept.



Neon has 8 electrons in the second (valence) shell, and 2 electrons in the inner (first) shell. Notice that we can number shells based on their distance from the nucleus. We can let the number "*n*" represent the number of the shell an electron is in. Thus, neon has 2 electrons in the *n*=1 shell and 8 electrons in the *n*=2 shell.

Name: ____ Period:______

5. Show how the core charge for neon was calculated.

6. Make two diagrams, similar to figures 3a and 3b, for the nitrogen atom.

We now consider two possible models for the sodium atom.

7. First we consider a model for sodium with 2 shells.
    a. Make two diagrams, similar to Figures 3a and 3b, for the sodium atom, assuming that the 11th electron goes into the second shell.

    b. What is the core charge for the sodium atom in question 7a?

    c. The IE_1 of neon is 2.08 MJ/mol. Predict whether the IE_1 for the sodium atom model in question 7a would be greater than, less than, or equal to 2.08MJ/mol. Explain your reasoning.

8. Next we consider a model for sodium with 3 shells.
    a. Make two diagrams, similar to Figures 3a and 3b, for the sodium atom assuming that the 11th electron goes into a new, third shell.

Name: ______________________________ Period:______

b. What is the core charge for the sodium atom model in question 8a?

c. Predict whether the IE_1 for the sodium atom model in question 8a would be greater than, less than, or equal to 2.08MJ/mol. Explain your reasoning.

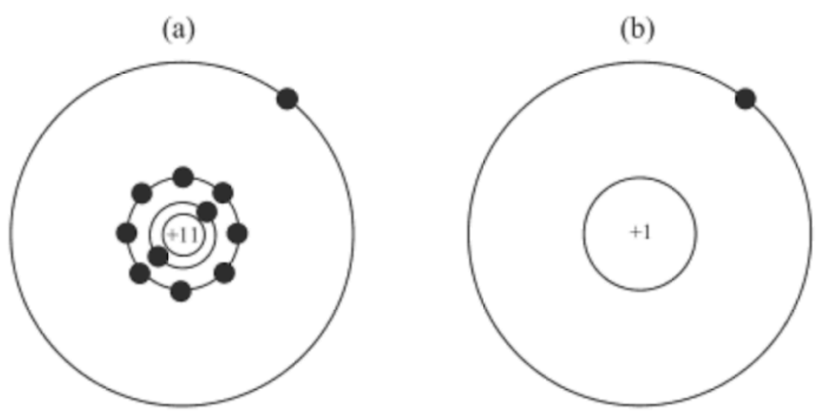
9. The observed IE_1 for sodium is 0.50MJ/mol. Use this datum to explain why the model for sodium suggested in question 8 is a better model than the one suggested in question 7.

Information

The IE_1 for sodium is 0.50MJ/mol, much less than the IE_1 for neon. This decrease in IE_1 from neon to sodium is analogous to (and similar in magnitude to) the decrease in IE_1 from helium to lithium. Also, note that the IE of sodium is even less than that of lithium (although only slightly so). Analogous to the conclusions we reached concerning the structure of the lithium atom, these results suggest that the eleventh electron in sodium should be placed in a third shell (n=3), at a slightly greater distance from the nucleus than the second shell (n=2) is for lithium. Thus, it appears that the n=2 shell can accommodate only eight electrons. (Recall that the n=1 shell holds only two.

Model 4: The Sodium Atom.

Figure 4: Diagram of a sodium atom using (a) the shell model and (b) the core charge concept.



10. How many electrons does sodium have in shell:
    a. n=1?
    b. n=2?
    c. n=3?

Name: ____ Period:_______

11. How does the core charge for sodium compare to the core charge for lithium?

12. Based on your answer to question 11 and the IE data given in Table 1 of CA4, is the radius of the valence shell of sodium larger, smaller, or the same as the radius of the valence shell of lithium? Explain your reasoning.

13. Consider the models of neon and sodium shown in Models 3 and 4. Explain how the core charges of sodium and neon are qualitatively consistent with the IE_1 data in Table 1 of CA4.

14. Use the core charge concept to propose an explanation for the increase of IE_1 from sodium (Z=11) through Ar (Z=18), as shown in Table 1 of CA4. Clearly state any assumptions that you make.

Model 5: The Shell Model and Ionization Energies.
Table 1: Atomic Properties of Various Atoms.

Element	Valence shell (*n*)	Number of Valence Electrons	Core Charge	IE_1 (MJ/mol)
H	1	1	+1	1.31
Li	2	1	+1	0.52
Na	3	1	+1	0.50
Rb				0.40
O	2	6	+6	1.31
S	3	6	+6	1.00
F	2	7	+7	1.68
Cl	3	7	+7	1.25

Name: ____ Period:_______

15. Identify the 3 elements in Table 1 that are shown to have the same core charge.

16. Referring to Table 1,
    a. What is the relationship between core charge and the number of valence electrons in an atom?

    b. In terms of the placement in the periodic table, what do the atoms with the same number of valence electrons have in common? Provide two specific examples from Table 1 to support your answer.

17.
    a. Identify the 3 elements in Table 1 that have valence shell n=2.

    b. Identify the 3 elements in Table 1 that have valence shell n=3.

    c. Locate the elements from parts a and b above on the periodic table. Describe the relationship between the valence shell of these atoms and their positions in the periodic table.

18.
    a. Based on its position in the periodic table, predict the valence shell, core charge, and number of valence electrons for rubidium and add these values to Table 1.

    b. Using the shell model and referring to the Coulombic Potential Energy relationship (equation in Model 1, CA3), explain clearly how the IE_1 for rubidium is consistent with your answer to part a.

19.
    a. Construct shell model diagrams of fluorine and chlorine that are consistent with the information in Table 1.

Name: ____ Period:_______

b. Within our model and referring to the Coulombic Potential Energy expression, explain why the IE_1 of chlorine is less than that of fluorine.

20. How does the core charge on a neutral atom change in moving from left to right across a row (period) of the periodic table?

21. WIthin our model and referring to the Coulombic Potential Energy expression, explain why the IE_1 increases from left to right across a row of the periodic table.

22. Based on its position in the periodic table, what is the valence shell and what is the core charge for carbon? Explain your reasoning.

Information

Consistent with the data in Table 1 of CA4, all of the atoms in Group 1A, the alkali metals, have a core charge of +1 and all of the atoms in Group 7A, the halogens, have a core charge of +7. In fact, for Groups 1A through 7A, the atoms in each group all have the same number of valence electrons, and that number is reflected by the group number. In all cases the IE decreases as we move down the group. This pattern is also observed in Group 8A, the Noble (or inert) gases. However, not all of the atoms we have examined in Group 8A have eight valence electrons (and a core charge of +8). Helium has only 2 electrons, a seeming violation of the pattern we have uncovered. The resolution of this apparent inconsistency is that although helium has only 2 valence electrons, its valence shell is *completely filled*. The same is true of neon, although for neon a filled valence shell has 8 electrons. Thus, we find that the structure of the elements using this shell model is reflected in the placement of the elements in the periodic table.