ChemActivity 5

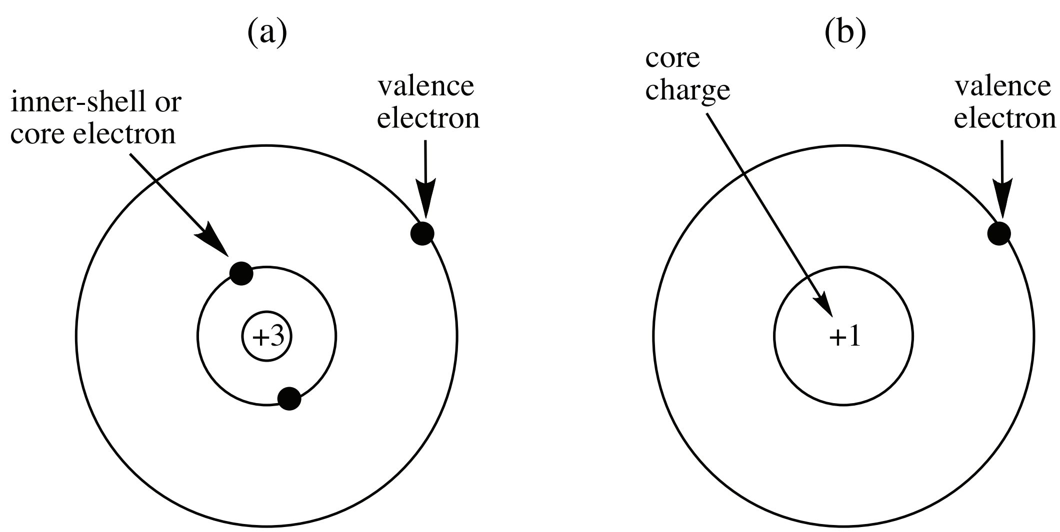
The Shell Model (II)

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

The electrons in the outermost shell of an atom are referred to as **valence** electrons. Electrons in shells closer to the nucleus are called **inner-shell** electrons. Thus, Li has one valence electron and two inner-shell electrons. H 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 Li atom in terms of core charge as shown in Figure 1.

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



Critical Thinking Questions

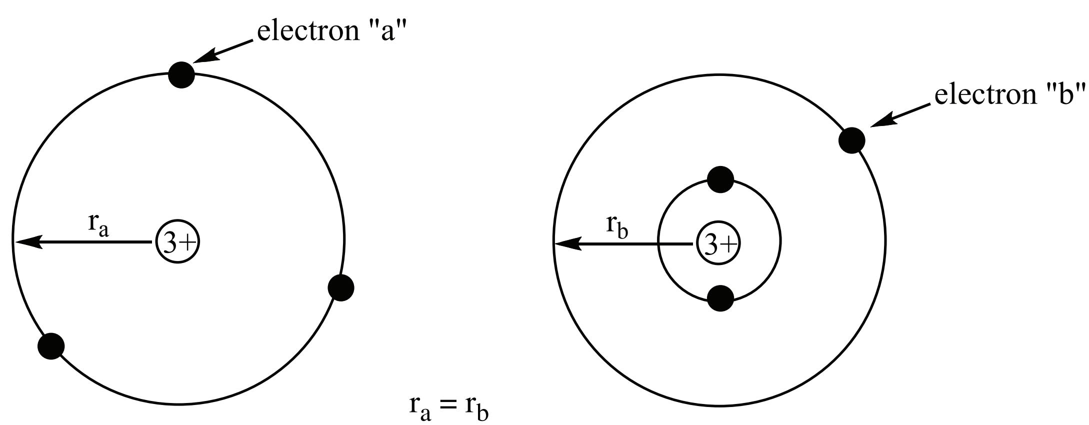
1. How many electrons are in the valence shell of a) H? b) Li? C) He?
2. How many inner-shell electrons are there in a) H? b) Li? C) He?
3. What is the core charge of Li?

Model 2: Core Charge and Electron-Electron Repulsion.

Notice that within the model of the Li atom, shown in Figure 1, 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 electron by the two inner-shell electrons. This dramatically decreases the overall force of attraction pulling the valence electron toward the nucleus.

Critical Thinking Question

4. Two possible models for arrangement of electrons in Li are shown below:

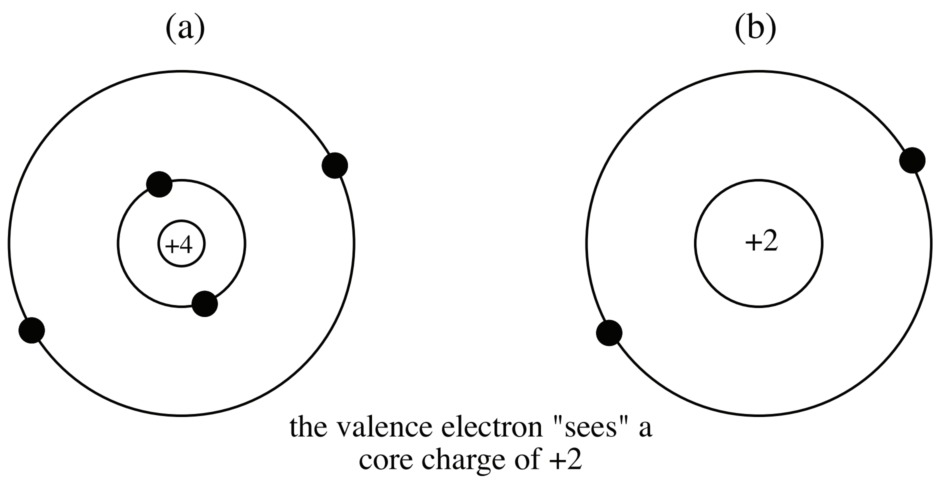


Explain why the IE_1 of electron "b" would be less than the IE_1 of electron "a".

Model 3: The Beryllium Atom.

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

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



Critical Thinking Questions

5. a) Why is the nuclear charge of Be "+4"?

   b) How many inner-shell electrons does Be have?

   c) How many valence electrons does Be have?

   d) Show how the core charge for Be was calculated.

   e) What is the relationship between the number of valence electrons and the core charge of a neutral atom?

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

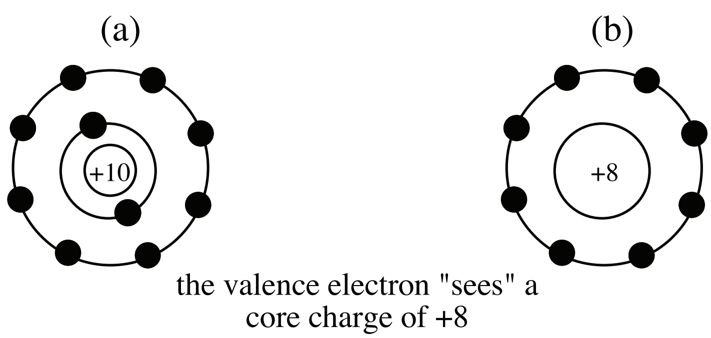
Information

As described above, the outer-shell valence electrons experience the charge of the core rather than the full charge of the nucleus. The inner electrons that surround the nucleus are said to *shield* the nucleus. In fact, because the valence electrons are all negatively charged, they repel each other also. Thus the net resulting 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. It is only an approximation, but it is adequate for our purposes.

Model 4: The Neon Atom.

Although there are some slight variations, in general there is an increase in ionization energy as the atomic number further increases up to Z = 10 (Ne). This is qualitatively consistent with an increase in core charge. (The slight variations will be addressed later.) There is no large drop in ionization energy to a value less than that of H, as we observed in going from He to Li, to indicate that a third shell is needed. This suggests that as we move from Be up to Ne, the number of electrons in the second shell increases.

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



Ne has 8 electrons in the second (valence) shell, and 2 electrons in the inner (first) shell. Notice that we can number the 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, Ne has 2 electrons in the $n = 1$ shell and 8 electrons in the $n = 2$ shell.

Critical Thinking Questions

7. Show how the core charge for Ne was calculated.

8. Make two diagrams, similar to Figures 3(a) and (b), for the nitrogen atom.

9. a) Make two diagrams, similar to Figures 3(a) and (b), for the sodium atom, assuming that the 11^{th} electron goes into the second shell.

   b) What is the core charge for the sodium atom in CTQ 9a?

   c) The IE_1 of Ne is 2.08 MJ/mole. Predict whether the IE_1 for the Na atom in CTQ 9a would be greater than, less than, or equal to 2.08 MJ/mole. Explain your reasoning.

10. a) Make two diagrams, similar to Figures 3(a) and (b), for the sodium atom, assuming that the 11^{th} electron goes into a new, third shell.

    b) What is the core charge for the sodium atom in CTQ 10a?

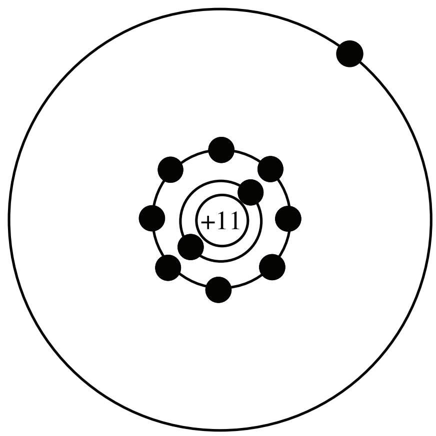
    c) Predict whether the IE_1 for the Na atom in CTQ 10a would be greater than, less than, or equal to 2.08 MJ/mole. Explain your reasoning.

11. The experimental IE_1 for Na is 0.50 MJ/mole. Use this datum to explain why the model for Na suggested in CTQ 10 is a better model than the one suggested in CTQ 9.

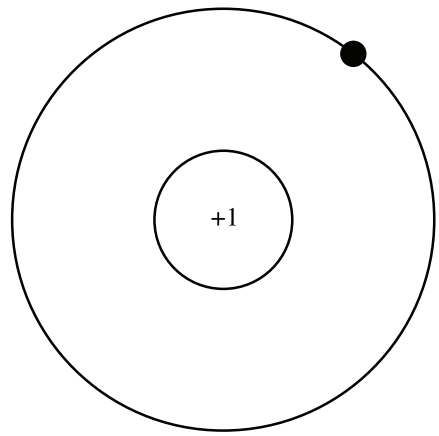
Model 5: The Sodium Atom.

Diagram of a Na atom using the shell model (a) and the core charge concept (b).

(a)



(b)



Critical Thinking Questions

12. How many electrons does Na have in shell $n = 1$? $n = 2$? $n = 3$?

13. How does the core charge for Na compare to the core charge for Li?

14. Based on your answer to CTQ 13 and the ionization energy data, Table 1 of **ChemActivity 4: Shell Model (I)**, is the radius of the valence shell of Na larger, smaller or the same as the radius of the valence shell of Li?

15. Consider the models of Ne and Na shown in Models 4 and 5. Explain how the core charges of Na and Ne are qualitatively consistent with the IE_1 data in Table 1 of **ChemActivity 4: Shell Model (I)**.

Information

The IE_1 for Na is 0.50 MJ/mole, much less than the IE_1 for Ne. This decrease is analogous to (and similar in magnitude to) that observed in going from He to Li. Note that the ionization energy of Na is only 0.50 MJ/mole, even less (although only slightly so) than that of Li. Analogous to the conclusions we reached concerning the structure of the Li atom, these results suggest that the eleventh electron in Na should be placed in a third shell ($n = 3$), at a slightly greater distance from the nucleus than the second shell is for Li. Thus, it appears that the $n = 2$ shell can accommodate only eight electrons. (Recall that the $n = 1$ shell holds only two.)

The pattern of ionization energies for the elements with Z = 11 to Z = 18 follows the trend we previously identified for Z = 3 to Z = 10: a general increase (with slight variations).

Critical Thinking Question

16. Use the core charge concept to propose an explanation for the increase of IE_1 from Na through Ar. Clearly state any assumptions that you make.

Information

As suggested by the data in Table 1 of **ChemActivity 4: Shell Model (I)**, 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 ionization energy 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 He has only 2 valence electrons, its valence shell is *completely filled*. The same is true of Ne, although for Ne 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.

Model 6: 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/mole)
H	1	1	+1	1.31
Li	2	1	+1	0.52
Na	3	1	+1	0.50
Rb				0.40
F	2	7	+7	1.68
Cl	3	7	+7	1.25

Critical Thinking Questions

17. Locate H, Li, and Na on the periodic table.

    a) Describe any relationship between the core charge of these atoms, the number of valence electrons, and their positions in the periodic table.

    b) Describe any relationship between the valence shell of these atoms and their positions in the periodic table.

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

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

18. Construct a shell model diagram of F that is consistent with the information in Table 1.

19. Locate F and Cl on the periodic table.

    a) Describe any relationship between the core charge of these atoms, the number of valence electrons, and their position in the periodic table.

    b) Describe any relationship between the valence shell of these atoms and their position in the periodic table.

    c) Within our model and referring to the Coulombic Potential Energy expression, explain why the IE_1 of Cl is less than that of F.

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

21. How does the core charge on the neutral atom change as we move from left to right across a row (period) of the periodic table?

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

Exercises

1. How many valence electrons are there in: a) C? b) O? c) N? d) Ne?

2. What is the core charge for: a) C? b) O? c) N? d) Ne?

3. Based on the information in Table 1 of **ChemActivity 4: Shell Model (I)**, estimate the ionization energy for Br. Explain your reasoning.

4. If a single electron is removed from a Li atom, the resulting Li^+ cation has only two electrons, both in the $n = 1$ shell. In this respect it is very similar to a He atom. How would you expect the ionization energy of a Li^+ cation to compare to that of a He atom? Explain your reasoning.

5. If a single electron is somehow added to a F atom, the resulting F^- anion has a total of 8 valence electrons in the $n = 2$ shell. In this respect it is very similar to a Ne atom. How would you expect the ionization energy of a F^- anion to compare to that of a Ne atom? Explain your reasoning.

6. Predict the order of the ionization energies for the atoms Br, Kr, and Rb. Explain your reasoning.

7. The radius of the outer shell in Li is larger than the radius of the inner shell. Which electron is harder to remove—the valence electron or one of the inner shell electrons? Explain.

Problems

1. Indicate whether each of the following statements is true or false and explain your reasoning.

   a) The core charge of Br is +7.
   b) Helium has the largest 1^{st} ionization energy.

2. Explain how the model of the structure of Be having the fourth electron in a third shell, further from the nucleus than any of the three electrons in Li, is *not* consistent with the experimentally obtained ionization energies.