What Does an Atom Look Like?

Why are we doing this?

The chemical properties of an atom are based on the number of outer-shell electrons. Thus, examining the atomic structure of an element can allow you to make predictions about various chemical properties including core charge, effective nuclear charge, and ionization energy. Additionally, an understanding of atomic structure can be used to interpret the significance of an elements position on the periodic table.

Your Learning Outcomes

You will be able to:

1. Predict the core charge of an atom.
2. Predict the number of valence electrons for an atom.
3. Use electronic structure to predict ionization energy or atomic radius.

The Plan

1. Assign roles*.
    a. ***Manager*** – This person will keep the team on task and provide direction to the group. This person is responsible for uploading the group's work to Gradescope. Make sure you make a note of everyone in the group. You must add everyone's name when submitting your answers to Gradescope.
    b. ***Spokesperson*** – This person will represent the group be responsible for speaking for the group to the rest of the class.
    c. ***Recorder*** – This person will be responsible for recording the team's answers to the Critical Thinking Questions in an organized and coherent manner.
    d. ***Analyst*** – This person will be responsible for critical analysis of the team's work (i.e., the Devil's Advocate). This person should make sure everyone understands what is happening before the group moves forward.
2. Complete the Critical Thinking Questions as a group.
3. Submit your team's work via Gradescope. Groups may choose to work in a Word document or write out their answers on a separate sheet of paper. All work must be upload to Gradescope as a PDF file.

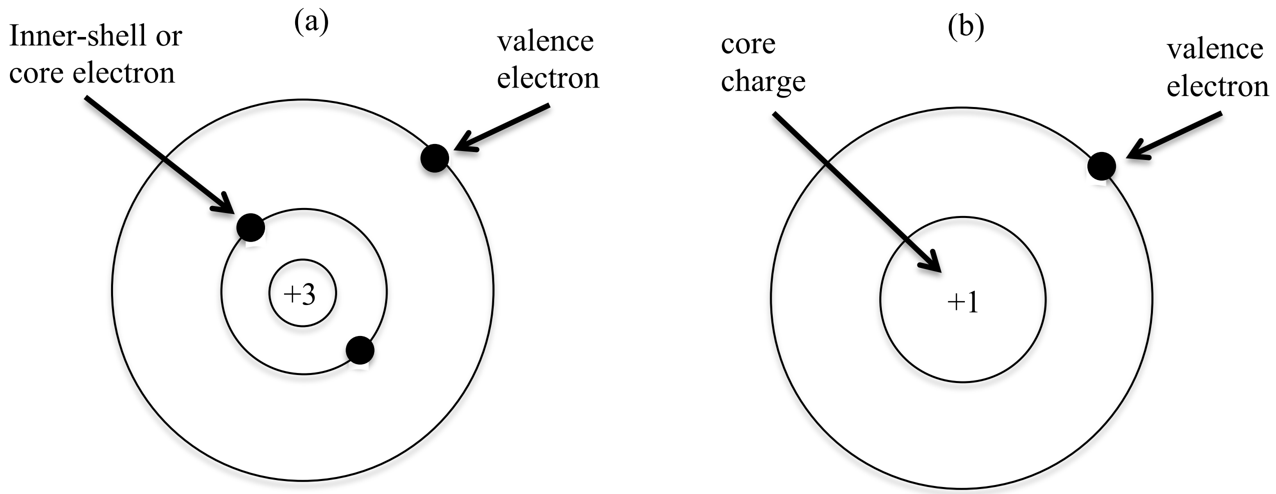
**Students may choose to complete this activity independently if they are unable to attend discussion due to illness or injury; in which case, the student must perform all roles and complete all aspect of the activity. To receive full credit, documentation as to the need for the absence from discussion must be included with the submission and your TA must be notified of the absence.*

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. This, 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 lithium atom using the shell model (a) and the core charge model (b)



Critical Thinking Questions

1. Complete the following table:

Atom	Total number of electrons	Number of valence shell electrons	Number of inner-shell electrons	Core Charge
H	1	1	0	+1
He	2	2	0	+2
Li	3	1	2	+1

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.

Information

Electrons in atoms are attracted to the positive charge of the nucleus. Thus, energy must be supplied (by some means) if an electron is to be pulled away from the nucleus. This energy is called the ionization energy (IE), i.e., the minimum energy required to remove an electron from a gaseous atom of that element. The first ionization energy (IE_1) is the energy to remove the first, outer-most electron.

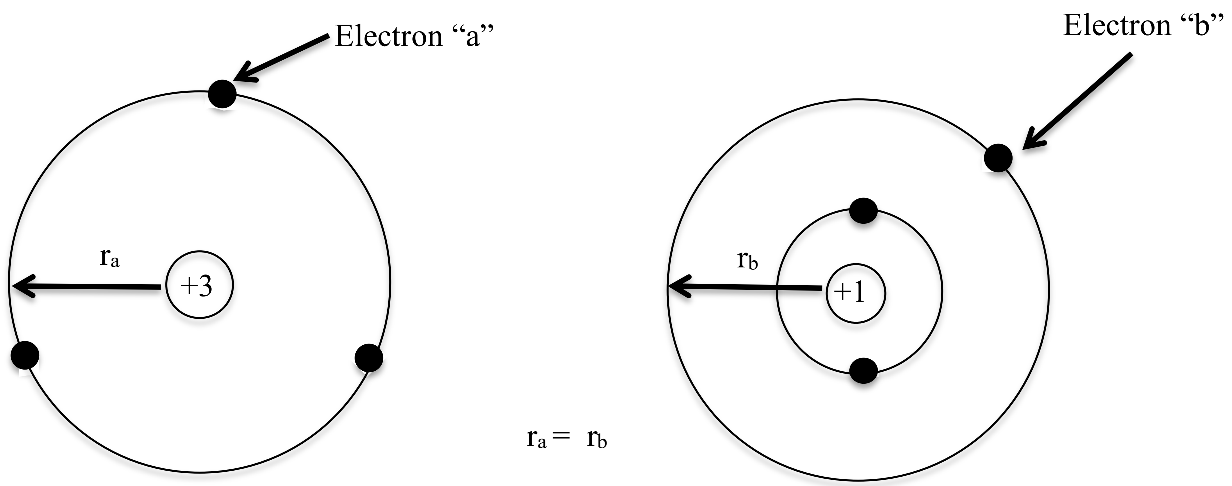
Table 1 below presents the experimentally measured ionization energies of the first 20 elements.

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 Question

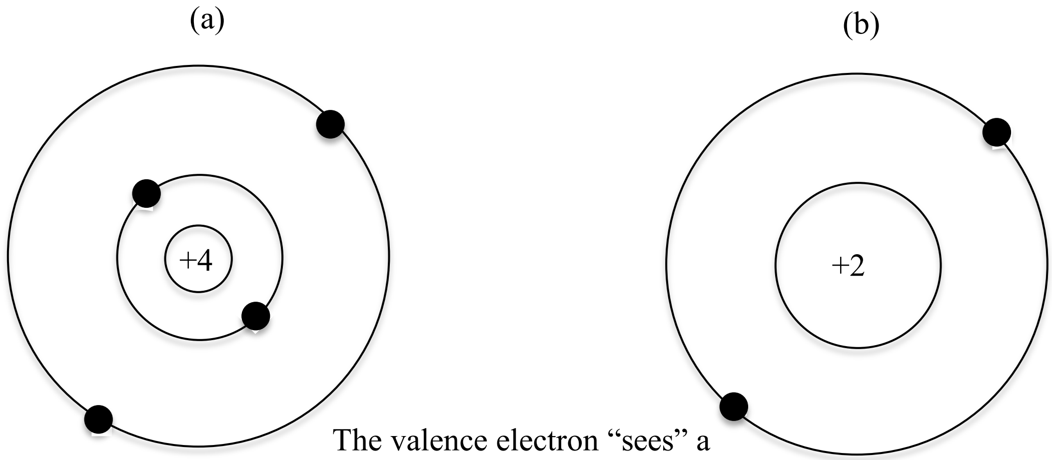
2. Two possible models for arrangement of the electrons in Li are shown below:



Explain why the IE_1 of electron "b" would be less than the IE_1 of electron "a".
Electron "b" experiences more electron-electron repulsion than electron "a" because electron "a" is farther from the other two electrons that electron "b". Therefore, the IE_1 of electron "b" would be less than the IE1 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.



The valence electron "sees" a core charge of +2

Critical Thinking Questions

3.

a. Why is the nuclear charge of Be "+4"?
Be has 4 protons in its nucleus.

b. How many inner-shell electrons does Be have?
Two

c. How many valence electrons does Be have?
Two

d. Show how the core charge for Be was calculated.
4 - 2 = +2

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?
The core charge is equal to the number of valence electrons for a neutral atom.

4. 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).
Be has a higher core charge (+2) than Li (+1) and a higher IE_1 than Li.

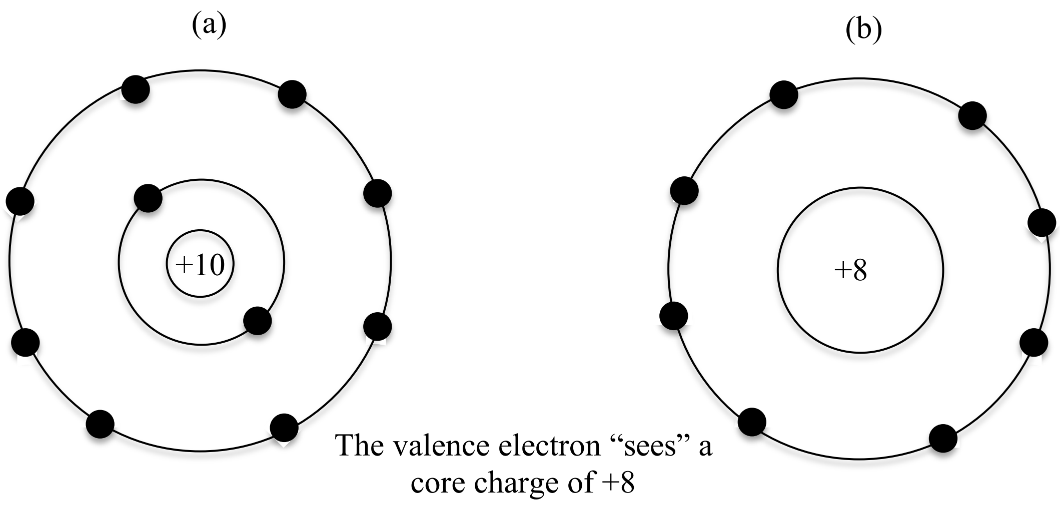
Information

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 towards 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) (refer to Table 1). 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).



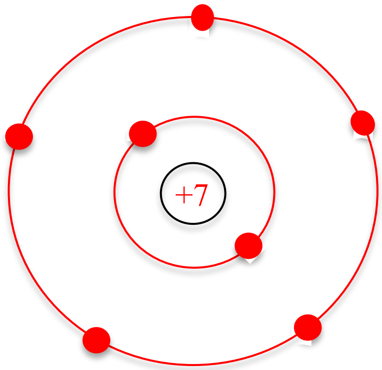
Ne has 8 electrons in the second (valence) shell, and 2 electrons in the inner (first) shell. Notice that we can number the shells based on their distance from the nucleus. We can let the number "n" represent the number of the shell an electron is in. Thus, Ne has 2 electrons in the n = 1 shell and 8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

Critical thinking Questions

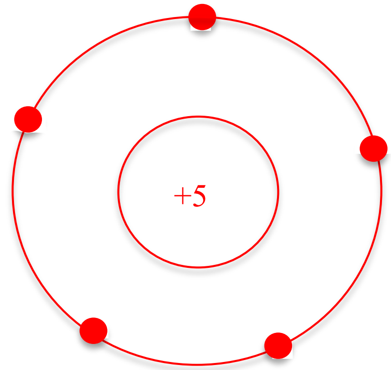
5. Show how the core charge for Ne was calculated.
   10 – 2 = +8

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

(a)



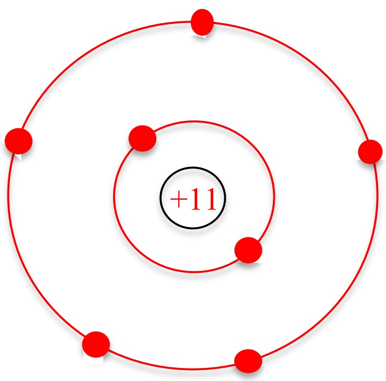
(b)



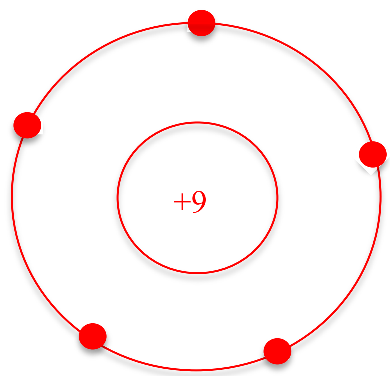
7.

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

(a)



(b)



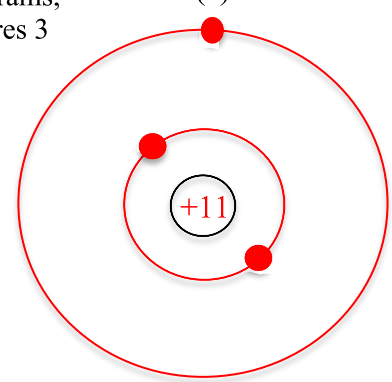
b. What is the core charge for the sodium atom in Question 7a?
11 – 2 = +9

c. The IE_1 of Ne is 2.08 MJ/mole. Predict whether the IE_1 for the Na atom in Question 7a would be greater than, less than, or equal to 2.08 MJ/mole. Explain your reasoning.
In this case, the Na atom would have the greater IE_1 because the core charge for Na would be +9 and for Ne +8. All of the electrons would be in the second shell and, therefore, about the same distance from the nucleus.

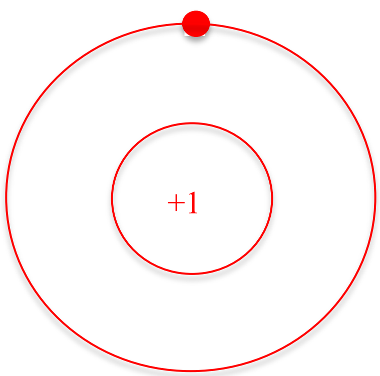
8.

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

(a)



(b)



b. What is the core charge for the sodium atom in Question 8a?
+1

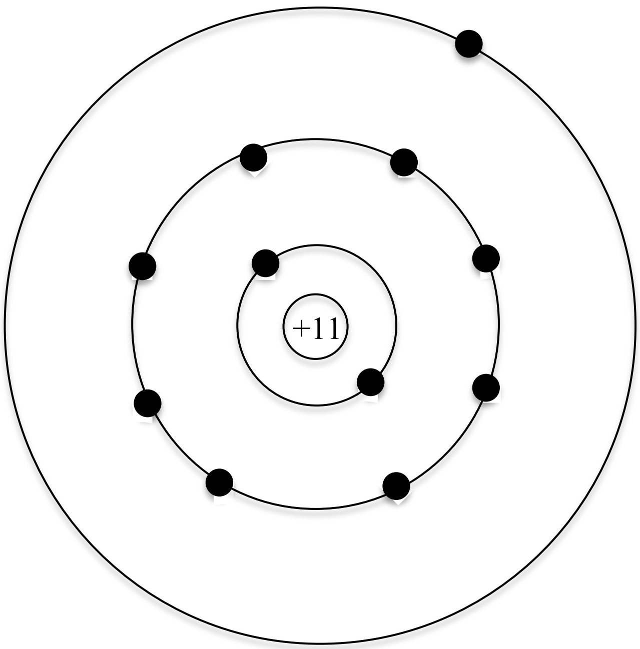
c. Predict whether the IE_1 for the Na atom in the Question 8a would be greater than, less than, or equal to 2.08 MJ/mole. Explain your reasoning.
Because the core charge of Ne is +8 and the core charge of Na is +1 (and because the outermost Na electron is farther from the nucleus) the IE_1 for Na should much less than 2.08 MJ/mole.

9. The experimental IE_1 for Na is 0.50 MJ/mole. Use the datum to explain why the model for Na suggested in Question 8 is a better model than the one suggested in Question 7.
The experimental IE_1 for Na is 0.50 MJ/mole. This is consistent with the model in Question 8

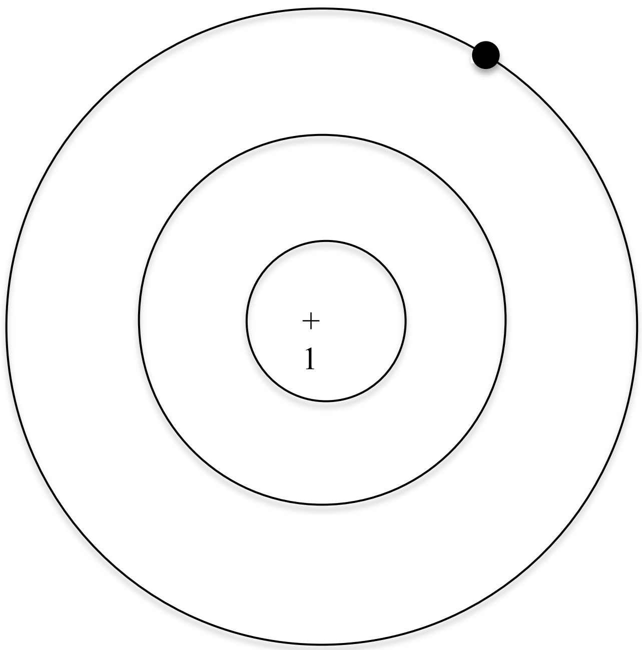
Model 5: The Sodium Atom.

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

(a)



(b)



Critical Thinking Questions

10. How many electrons does Na have in shell n = 1? n = 2? n = 3?
2, 8, 1

11. How does the core charge for Na compare to the core charge for Li?
Both have a core charge of +1.

12. Based on your answer to Question 11 and the ionization energy data in Table 1, is the radius of the valence shell in Na larger, smaller, or the same as the radius of the valence shell of Li?
The radius of the valence shell of Na is larger than the radius of the valence shell of Li because they both have a core charge of +1 and Na has the lower IE_1.

13. 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.
Na has a core charge of +1 and Ne has a core charge of +8. Na should have a much lower IE_1, which it does. This is consistent with the experimental data.