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## Part A. Coulomb's Law and the Ionization Energy of Electrons

Analysis of atomic emission spectra leads to the conclusion that electrons in an atom reside in quantized energy levels or shells. The shells have discrete energies based on the distance separating the electrons from the nucleus and the charge of the nucleus. These energies may be qualitatively compared using Coulomb's law, which states that the force (F) experienced by two charged objects,  $q_1$  and  $q_2$ , is inversely related to the square of the distance (r) separating them (Equation 2). If the two objects have opposite charges, then the force between them is attractive; if the charges are the same then the force is repulsive.

$$F \propto \frac{q_1 q_2}{r^2}$$
 Equation 2

1. Rank the diagrams A, B and C representing the distances between a proton (+) and an electron (-) in order of smallest force of attraction to largest. Explain how you made your determination.



- 2. Which electron in diagrams A-C would require the most energy to be removed from the vicinity of the proton?
- 3. If the distance between the proton and electron in diagram C were increased to 0.60 nm, would you predict the force of attraction to be stronger or weaker than the original?
- 4. Consider the following diagrams representing different numbers of protons in an atomic nucleus. Which electron would require the most energy to be removed?



5. Describe the types of forces experienced by electrons X and Y in the following diagram.



6. Which electron would require more energy to be removed from the system of charges?

Consider the following "shell diagram" for a hypothetical atom (Figure 2).





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- 7. Which electrons in Figure 2 are in the same energy level?
- 8. What type of force is experienced between the electrons and the nucleus?
- 9. What type of force is experienced between different electrons in Figure 2?
- 10. Compare the force of the nucleus on the electrons in both shells in Figure 2. Based on Coulomb's law, which electron(s) experience a greater force? Explain.
- 11. Predict which electron(s) would require the least amount of energy to be removed (ionized) from the atom. Explain your reasoning.
- 12. Suppose photoelectron spectroscopy yielded ionization energy values of 0.76 MJ/mol and 5.25 MJ/mol for the electrons in this hypothetical atom. How much energy, in MJ, is required to remove electron B from one mole of atoms? *Note:* 1 MJ = 1 Megajoule =  $1 \times 10^6$  J.

## Photon Energy 25 MJ/mole $A^+$ $e^-$ KE = 13 MJ/mole



- 1. Figure 3 represents the basic physical process that takes place in photoelectron spectroscopy. What is the energy per mole of the photon in this example?
- 2. What is the kinetic energy per mole of the photoelectron that is released from A?
- 3. Determine the ionization energy per mole of the ejected electron.
- 4. The photoelectron spectrum is usually plotted as shown below in Figure 4 for A. *Ionization energy* is on the *x*-axis versus *signal intensity* on the *y*-axis. Note the position of zero on the *x*-axis. (*a*) Write a sentence describing how the value of the ionization energy increases along the *x*-axis in a photoelectron spectrum. (*b*) Which direction on the *x*-axis corresponds to greater kinetic energy of an emitted photoelectron?



Figure 4. A simulated photoelectron spectrum.

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- 5. What determines the position of the peak in the spectrum? What is the numerical value of the peak for atom (element) A?
- 6. How many energy levels are represented by the photoelectron spectrum in Figure 4? Explain your reasoning.
- 7. Is it possible to determine how many electrons are present in A based on this spectrum? Explain.
- 8. The simulated photoelectron spectrum for a second hypothetical element is shown below. What does the number of peaks indicate about the energy levels for the electrons in this element?



Figure 5. Simulated photoelectron spectrum.

- 9. What are the ionization energies for the electrons in Figure 5?
- 10. Which ionization energy value corresponds to an electron that is closer to the nucleus?
- 11. Compare the peak heights for the signals in this spectrum. Predict the relative number of electrons per atom originating from each energy level.
- 12. Complete the following shell diagram for this hypothetical element based on the photoelectron spectrum in Figure 5.



## Part C. Photoelectron Spectra (PES) and Electron Configurations of the Elements

Table 1 summarizes PES data for elements 1-4 (hydrogen through beryllium).

Element	Ionization Energy (MJ/mol)		
	Peak A	Peak B	
Н	1.31		
He	2.37		
Li	6.26	0.52	
Be	11.5	0.90	

Table 1.

- 1. Compare the ionization energy values for hydrogen and helium. What is the main factor accounting for the difference in ionization energy of these two elements?
- 2. Helium has two electrons but only one peak in its photoelectron spectrum. Explain.
- 3. For each element in Table 1, the electrons giving rise to Peak A are all in the same energy level (n = 1). Explain how the charge on the nucleus and the distance of these electrons from the nucleus might (or might not) account for the trend in these ionization energy values for elements 1-4.
- 4. For each element, identify the peak corresponding to the first (lower) ionization energy. Account for the difference in energy for the first ionization of elements 1–4.
- 5. Compare the ionization energy for Peak A in the photoelectron spectrum of hydrogen versus Peak B for lithium. Draw simple shell diagrams to illustrate the difference in ionization energy for these peaks.



Hydrogen



6. The photoelectron spectrum of lithium is shown in Figure 6. Identify the peak representing the first ionization energy of lithium.



Figure 6. Photoelectron spectrum of lithium.

- 7. Compare the energy and relative height of the peaks in Figure 6. Write out the accepted electron configuration for lithium and assign the peaks in the PES of lithium to these atomic orbitals.
- 8. Consider the element boron with five electrons in a neutral atom. Predict the number of peaks, and their relative height, in the photoelectron spectrum of boron.
- 9. The actual photoelectron spectrum of boron is shown below. Describe any similarities and differences in the information obtained from this spectrum with the predictions you made in Question 8.



Figure 7. Photoelectron spectrum of boron.

- 10. The n = 2 energy level of an atom consists of two subshells (2s and 2p orbitals). What does the presence of a third peak in the PES of boron indicate about its electronic structure? Use the terms shells and subshells in your answer, and be as specific as possible concerning the difference in energy of the three peaks, as well as their relative height.
- 11. Assign each peak in Figure 7 to electrons and atomic orbitals in the accepted electron configuration of boron.

- 12. The 1s and 2s orbitals can each accommodate two electrons. How many electrons can occupy the 2p subshell in an atom?
- 13. Complete Table 2 to predict the number of peaks, and the relative number of electrons, for the remaining elements in row 2 of the periodic table. Arrange the peaks from lowest to highest ionization energy to show the relative number of electrons.

Table 2.

Element	Atomic Number	Number of Peaks	Relative Number of Electrons (from lowest to highest IE)
Li	3	2	1:2
Be			
В	5	3	1:2:2
С			
N			
0			
F			
Ne			

14. Compared to the elements in Table 2, the PES of sodium (element 11) contains a new, fourth peak. Would you expect this peak to have a lower or higher ionization energy value than the lowest IE peak for neon? Explain based on the arrangement of elements in the periodic table and the shell structure of atoms.

Table 3 summarizes atomic orbital assignments for the ionization energy values obtained from the photoelectron spectra of elements 11–20.

Element	Ionization Energy (MJ/mol)						
	1s	2s	2p	3s	3p	4s	
Na	104	6.84	3.67	0.50			
Mg	126	9.07	5.31	0.74			
Al	151	12.1	7.19	1.09	0.58		
Si	178	15.1	10.3	1.46	0.79		
Р	208	18.7	13.5	1.95	1.06		
S	239	22.7	16.5	2.05	1.00		
Cl	273	26.8	20.2	2.44	1.25		
Ar	309	31.5	24.1	2.82	1.52		
K	347	37.1	29.1	3.93	2.38	0.42	
Ca	390	42.7	34.0	4.65	2.90	0.59	

Table 3.

15. Based on the ionization energy data in Table 3, which orbitals appear to be closer in absolute energy—a 1s and 2s orbital, or a 2s and 3s orbital? Explain based on energy as a function of distance from the nucleus.

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- 16. The potential energies of electrons in an atom are always negative, meaning they are more stable than isolated or "free" electrons. This leads to an apparently contradictory statement that "electrons that are higher in energy have lower ionization energies." Write a short 1–3 sentence explanation for ionization energy that eliminates potential confusion about these terms.
- 17. The relative energies for the atomic orbitals of Mg are shown below. Draw lines to show the approximate relative energies of the 1s, 2s, 2p, 3s, and 3p orbitals of Al.



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