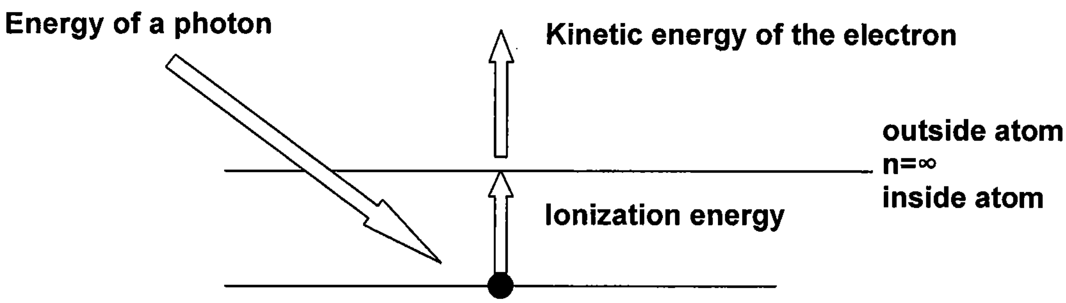
Photoelectron Spectroscopy (PES) and Electron Configurations

This activity is modified from Chemistry: A Guided Inquiry (3/e) by R.S. Moog and J.J. Farrell, Wiley, 2006.

A photon hits an electron, ejecting it from an atom with a certain amount of kinetic energy.

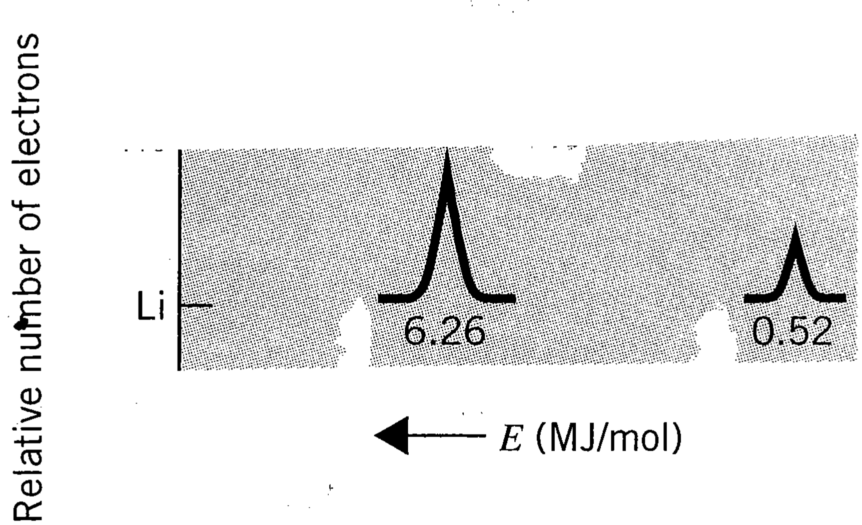


Q1) How is the ionization energy (IE) of the atom and the kinetic energy (KE) of the ejected electron related to the energy of the photon? Give an equation (assume energy is conserved).

Information

When a photon hits an electron, the electron has enough energy to leave the atom (ionization energy) plus some extra energy which it uses for kinetic energy. This kinetic energy can be measured using Photoelectron spectroscopy (PES). If the energy of the incoming photon is known, and the kinetic energy of the outgoing electron is measured, then the ionization energy of an atom can be calculated.

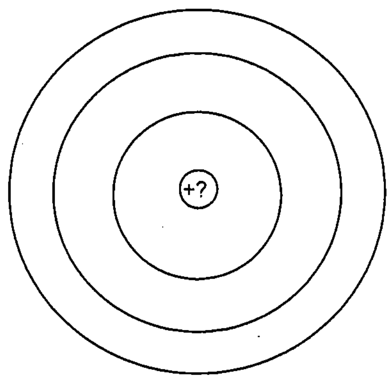
Model 1: Photoelectron spectrum of Lithium



Q2) Based on the number of peaks in Model 1, how many shells are in Li?

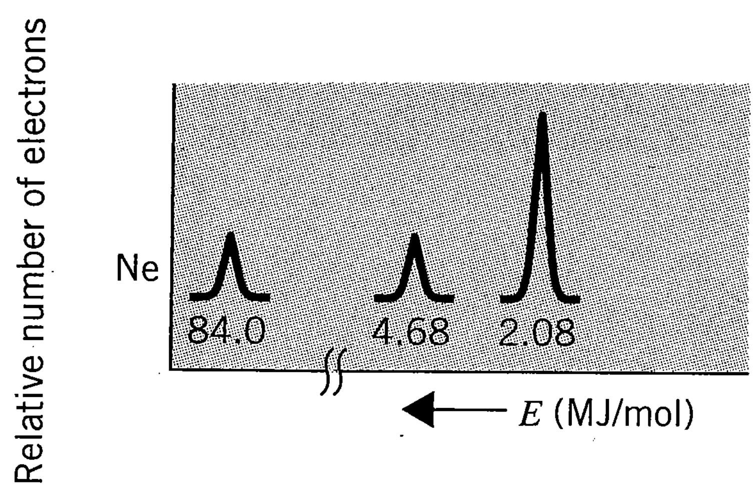
Q3) What does the height (area) of a peak tell you about the shells?
What does it tell us about Li?

Q4) Use the template below to complete a shell model diagram of neon. Fill it in with the nuclear charge and electrons.



Q5) How many peaks do you predict in the photoelectron spectrum of Neon?

Model 2: Photoelectron spectrum for Neon



Q6) Which peak corresponds to the first shell? (Look at the ionization values that make sense.)

Q7) If there are ten electrons total, label the peaks with the number of electrons they represent.

In Q5, you should have predicted that based on the Shell Model of Neon, there would only be two peaks—one for each shell (n=1 & 2). However, in Model 2 you see there are actually three peaks! The first shell is closest to the nucleus and has the highest IE. The other two peaks are closer in IE to each other; they are the result of splitting the second shell into two subshells. One subshell contains two electrons and the other contains six.

Q8) Subshells are labeled s, p, d, f

a) Which kind of subshell (s, p, d, f) holds 2 electrons max?

b) Which kind of subshell (s, p, d, f) holds 6 electrons max?

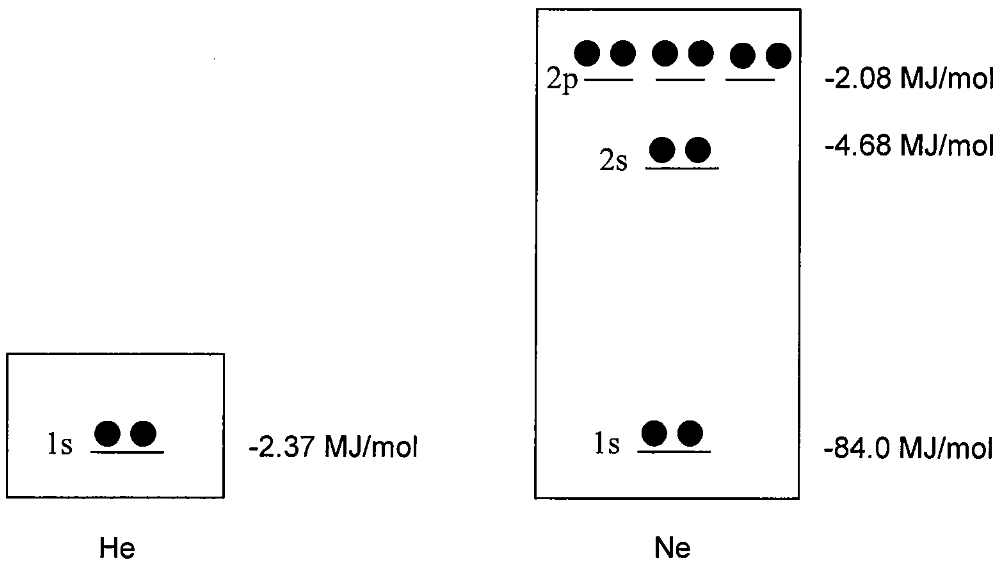
c) An orbital is given a shell # (1, 2, etc...) and a subshell letter (s, p, d, f).
Label each peak in Model 2 with the correct orbital designations (1s, etc...)

Q9) Which element gives this photoelectron spectrum? Explain.

Exercise: Sketch the photoelectron spectrum for Argon. (Ionization energies in MJ/mol for Ar: 1s (309); 2s (31.5); 2p (24.1); 3s (2.82); 3p (1.52). Don't forget to get the correct relative areas for each peak. Always label your axes.

Model 3: Energy Diagrams from PES

(Obviously, energies are not drawn to scale!)



In the energy diagrams, the lowest energy orbitals are at the bottom and the higher energy orbitals are at the top. Electrons in the lower energy orbitals are more stable than those in the higher energy orbitals. There's only one "s" orbital, but there are three "p" orbitals in a given subshell.

Q10) Based on the energy diagrams in Model 3 and your sketch of the Ar spectrum, draw an energy diagram for Ar (in the same fashion as in Model 3).

Q11) An electron configuration shows the shell number (1, 2, etc..) the subshell designation (s, p, d, f) and the number of electrons occupying the orbitals. Example: Neon is $1s^22s^22p^6$ since two electrons occupy 1s, two electrons occupy 2s, and six electrons occupy the 2p orbitals.

Write the electron configuration for all elements from Na to Ar.

a) In the electron configurations given above, circle the portion that shows the valence (outermost) electron(s).

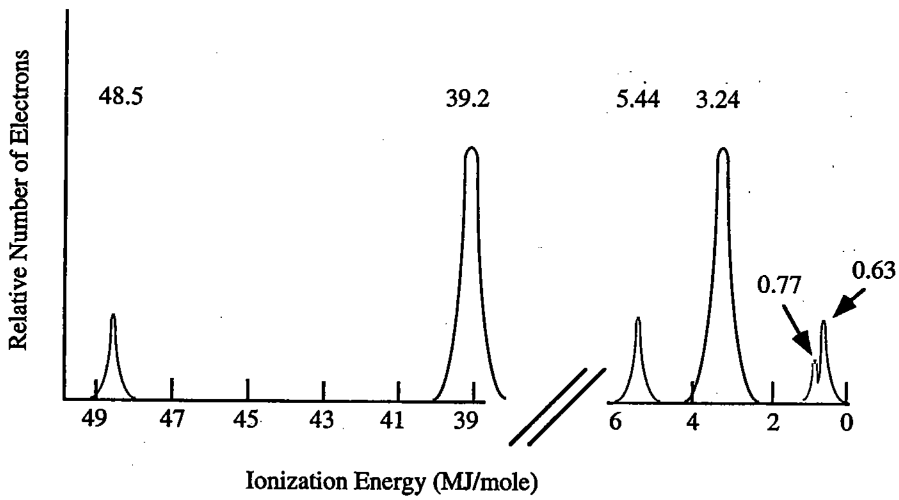
b) Is there are relationship between the valence electrons and the position of the element in the periodic table?

c) Write the electron configuration for Na^+, Mg^{2+}, Al^{3+}. What do they have in common?

d) Write the electron configuration for P^{3-}, S^{2-}, Cl^-. What do they have in common?

Model 4: Simulated PES of Scandium

(The 1s peak occurs at 433 MJ/mole and is not shown in this spectrum.)



Q12) Assign each peak in the spectrum with an orbital designation. Explain why the peak at 0.77 MJ/mol should be assigned as 3d rather than 4p.

a) According to the spectrum above, which orbitals get filled first, 4s or 3d?

b) According to the spectrum above, which electrons are removed from an atom first, 4s or 3d?

Model 5: Periodic Table

Look at Figure 7.13 (page 296) in Moore, Stanitski, Jurs. This is a strange shape! This is what the periodic table really looks like (the kind you're used to is just a condensed version!)

Do you notice that there are 4 kinds of "blocks" (s, p, d, f)? This figure walks you through the lowest energy orbitals (starting with 1s) to higher orbitals (in the order of increasing atomic number, which is left to right, then top to bottom) in the order that they are filled.

Q13) Based on the form of the periodic table (as it is in Figure 7.13), how many electrons does it take to fill an "s block"? How about a "p" block? "d" block? "f" block?

Q14) Predict the electron configuration of Gallium (Ga)

Q15) For Q14, did you get: $1s^2 2s^2 sp^6 3s^2 3p^6 4s^2 3d^{10} 4p^1$?

There is a shortcut you can use. Included in the configuration of Ga is the **noble gas that precedes it**, Ar (which is $1s^2 2s^2 sp^6 3s^2 3p^6$). The shortcut allows you to write for Ga:

Noble gas shorthand for Gallium: [Ar] $4s^2 3d^{10} 4p^1$

It sure saves time! It also shows you which electrons are the core electrons ($1s^2 2s^2 sp^6 3s^2 3p^6$) and the valence electrons ($4s^2 3d^{10} 4p^1$)

Try the noble gas shorthand configuration for Tin (Sn).

Q16) In terms of electron configurations and the periodic table (as shown in Figure 7.13): Are elements in the same period (row) more similar to each other, or are elements in the same group (column) more similar to each other?

Exercises

This material is not covered in your textbook. A reference material will be placed on the website if you need assistance with this material.

1. Place the following in order of increasing energy to remove an electron from the 1s energy level: C, Pt, Ba, Ne, Zn, Gd

2. Make a rough sketch of the photoelectron spectrum of vanadium (use scandium example as a model). Indicate the subshell that gives rise to each peak and the relative height of each peak.

3. Provide the electron configuration for: P, P^{3-}, Ba, Ba^{2+}, S, S^{2-}, Ni, Zn

4. As atomic orbitals are filled, the 6p orbitals are filled immediately after which of the following orbitals? 4f, 5d, 6s, 7s

5. Identify the 2 elements whose simulated photoelectron spectra are shown below: