

Question: Do all electrons in the same level have the same energy?

From the Shells Activity, one important conclusion we reached based on the first ionization energy experimental data is that electrons in higher shells require less energy to remove. We have experimental data that relates energy required to remove an electron depending on the shell the electron occupies. (In which shell does an electron require more energy to remove? An electron in the second shell or the fourth shell?) An interesting question we could ask, that can not be answered from the experimental data of the first ionization energy is, do all electrons in the same shell require the same amount of energy to remove? We can answer this question if we look at photoelectron spectroscopy (PES) data for the atoms.

In a photoelectron spectroscopy experiment any electron can be ionized when the atom is excited. Like the first ionization only one electron is removed from the atom, however in the PES experiment it can be any electron, not just the electron that requires the least amount of energy.

Additional examples of photoelectron spectra data are available at <http://www.chem.arizona.edu/chemt/Flash/photoelectron.html>. Open this web page. To display the first spectrum, click on hydrogen in the periodic table.
Bodner, Spencer and textbook. 5th Edition Wiley and Sons.

<http://www.cbc.arizona.edu/rss/pes/tutorials/tutorials.htm>

It is recommended that you have the Shells Activity for reference while working on this activity. The Shells Activity is available at http://genchem1.chem.okstate.edu/CCLIEMD09/Shells_Activity.pdf

Look at the PES spectrum for Hydrogen shown in Figure I.

1. The label on the y -axis is energy and the units are in megajoules(M J mol^{-1}). What does the x -axis depict?

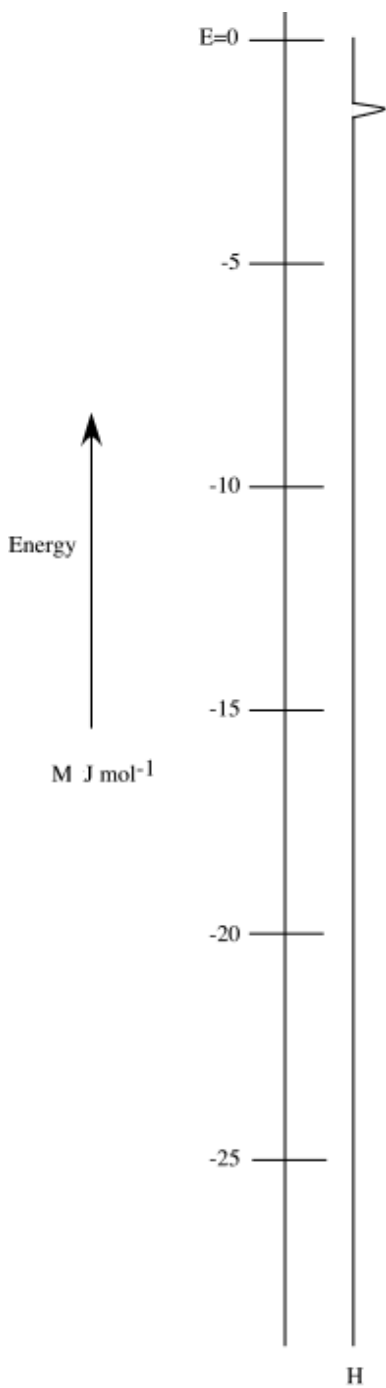


Figure I.

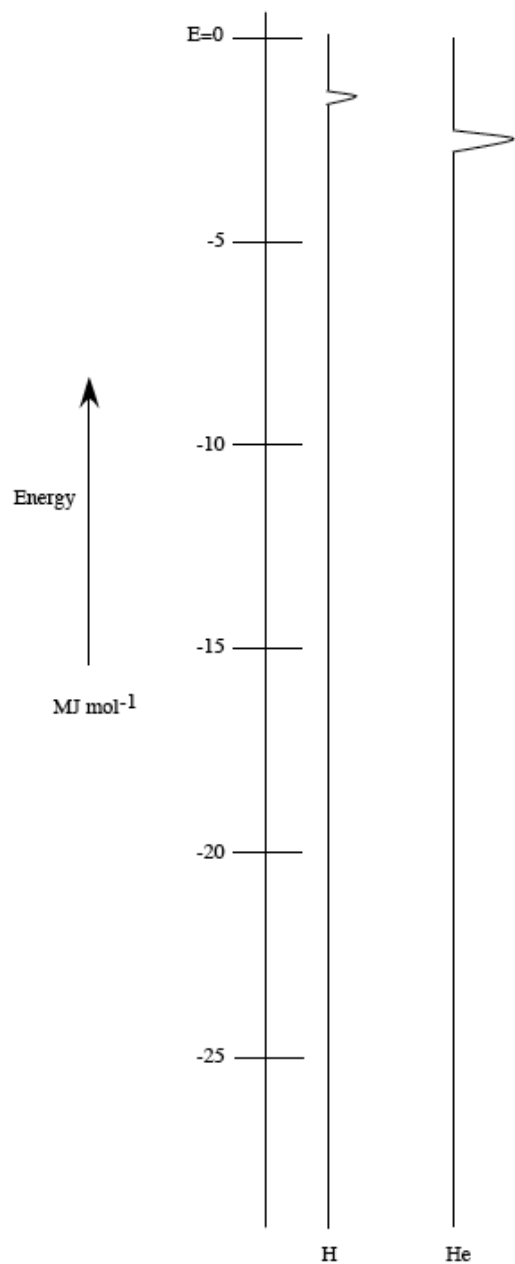


Figure II: PES for Hydrogen and Helium

4. Look at the PES in Figure II. and compare it to the prediction from the previous question. Describe what you see and the conclusion(s) you reached? (Note: be sure to comment about the relative energy of the peak(s) and the number of electrons for each peak in the PES for He and the PES for H.)

Note: The PES spectra show the energy of every electron in an atom, while the ionization energy information only provides the energy of the electron in the atom that is the easiest to remove. The PES spectrum of hydrogen and helium shows that

the electrons in helium are at lower energy, therefore requiring more energy to remove each electron.

5. The next element is lithium.
 - a. How many electrons does lithium have and what shells do those electrons occupy?

 - b. Before looking at the PES for lithium predict what you believe the spectrum would look like? Note: you do not have to predict the exact energies of each electron but you can make reasonable estimates based on the first ionization energy for lithium and the PES for helium. Use the data for lithium from Shell Activity to help make your prediction.

When the students predict there are two peaks, then ask what is the relative energy of each peak and how do the peaks integrate for numbers of electrons.

In software, enter the name of the element...lithium, then the software asks how many shells are required for the total number of electrons in lithium? Student responses '2', then the software asks How many electrons in each shell, and the energy required to remove the electrons in each shell. After the student does this prediction the actual PES for lithium is drawn and the student is asked to compare their prediction to the actual PES spectrum.

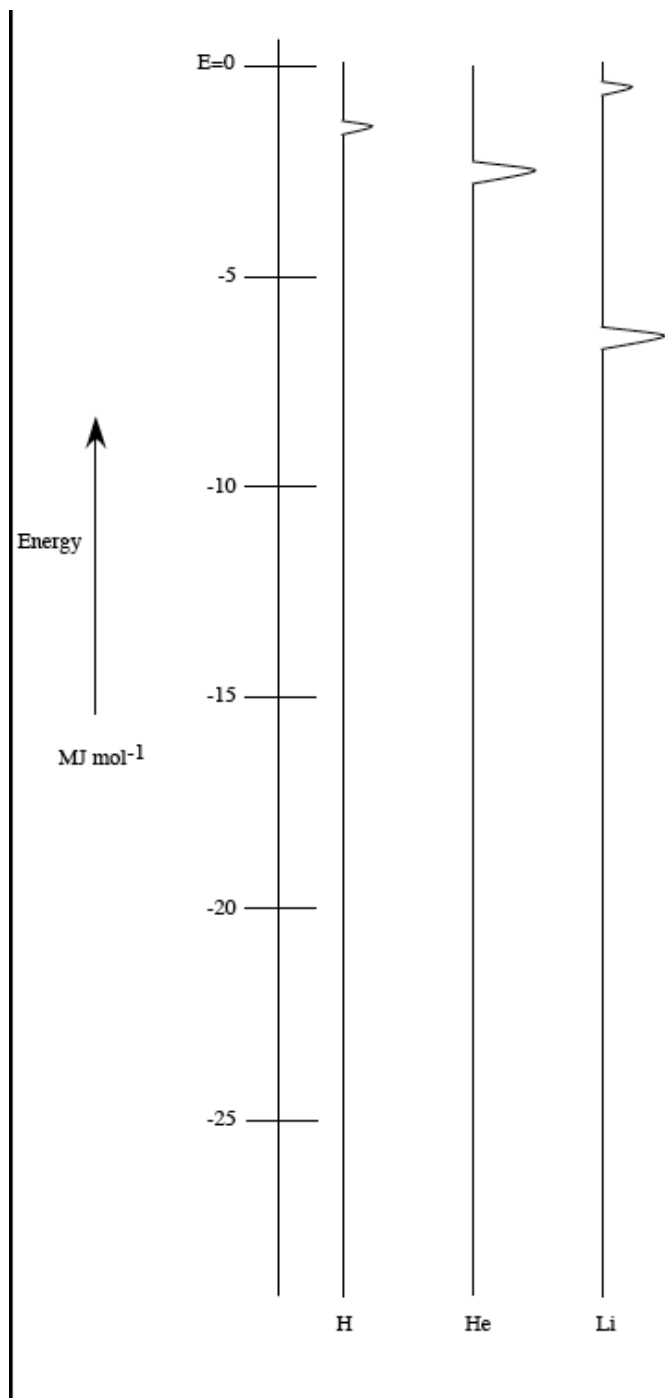


Figure III PES for H, He and Li

5. Look at the PES in Figure III. and compare it to the prediction from the previous question. For each peak in the PES identify the shell the electrons represented by that peak occupy. Describe what you see and the conclusion(s) you reached? (Note: be sure to comment about the relative energy of the peak(s) and the number of electrons for each peak in the PES for Li.)
6. The next element is beryllium.

- a. For the PES for beryllium predict how many peaks, the number of electron for each peak and the estimate the relative energies. How many electrons does beryllium have and what shells do those electrons occupy?

NOTE: Do we want to add the subscript number of protons on the symbols of the elements in the PES spectrum?

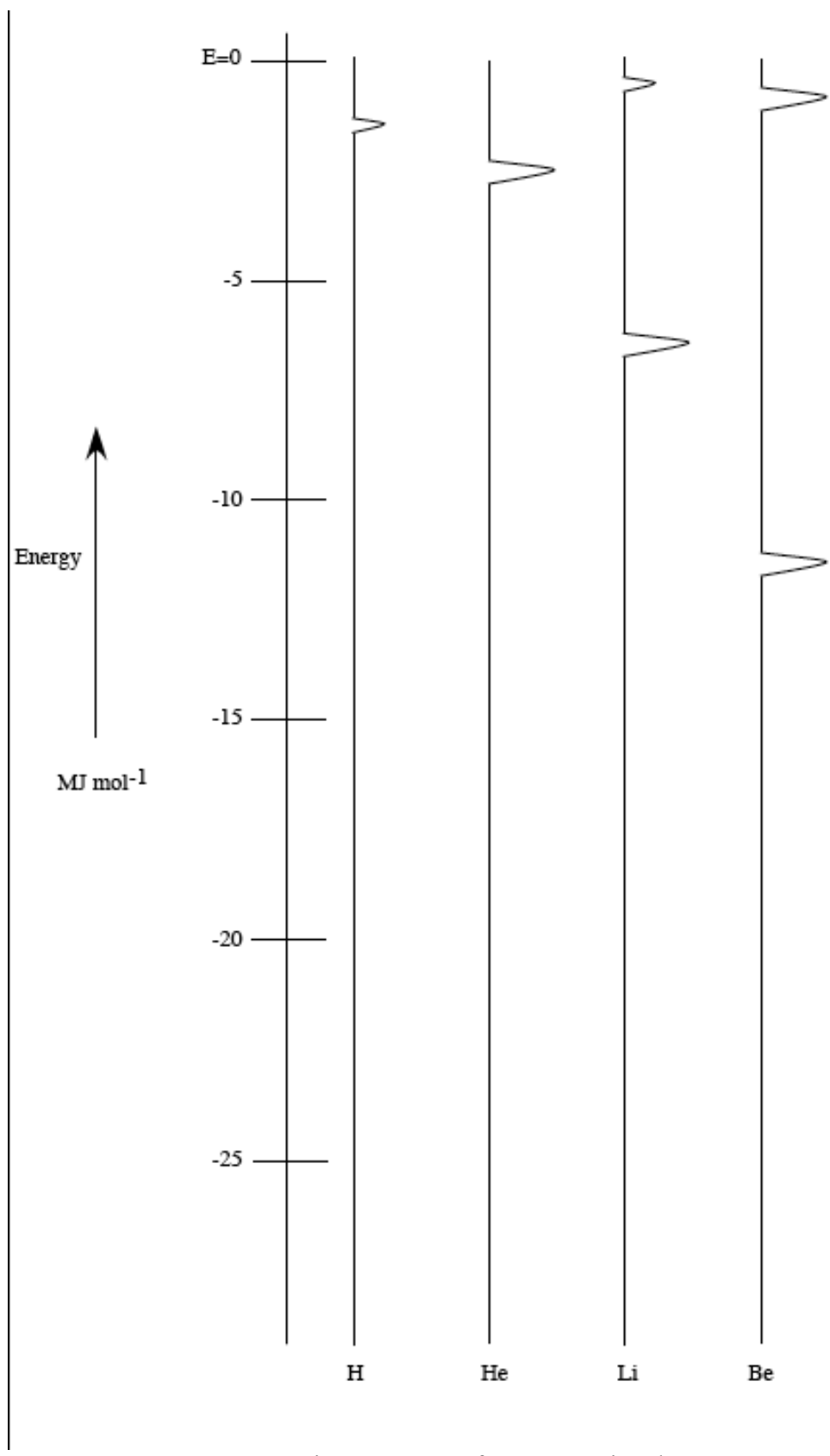


Figure IV. PES for H, He, Li and Be

7. The next element is boron.
- How many electrons does boron have and what shells do those electrons occupy?

 - For the PES for boron predict how many peaks, the number of electron(s) for each peak and estimate the relative energies.

 - Describe the experimental PES for boron. Briefly describe how to interpret the PES for boron.

NOTE: The PES for boron has three peaks! The peak at lowest energy has two electrons so we see the electrons for that peak are the electrons in the first shell. Boron has three electrons in the second shell, but according to the PES those three electrons have different energies, although relatively close together. One interpretation of this observation is that the three electrons in the second shell occupy two 'subshells' of different energy. So the idea of subshells within shells must be introduced to understand the different energies of the three electrons. If the PES had shown two peaks, one integrating for two electrons and one integrating for three electrons the concept of a subshell would not be required.

8. Predict what changes in the PES you would expect to see going from carbon to neon? Look at the PES for these second period elements.

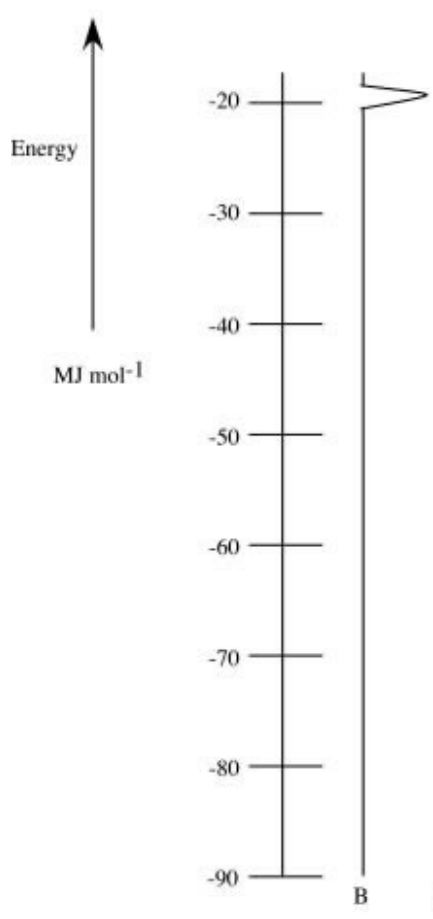
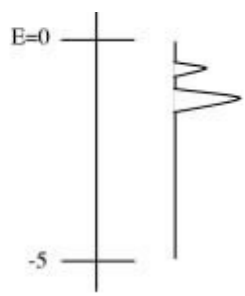


Figure IV. PES for Boron (B)

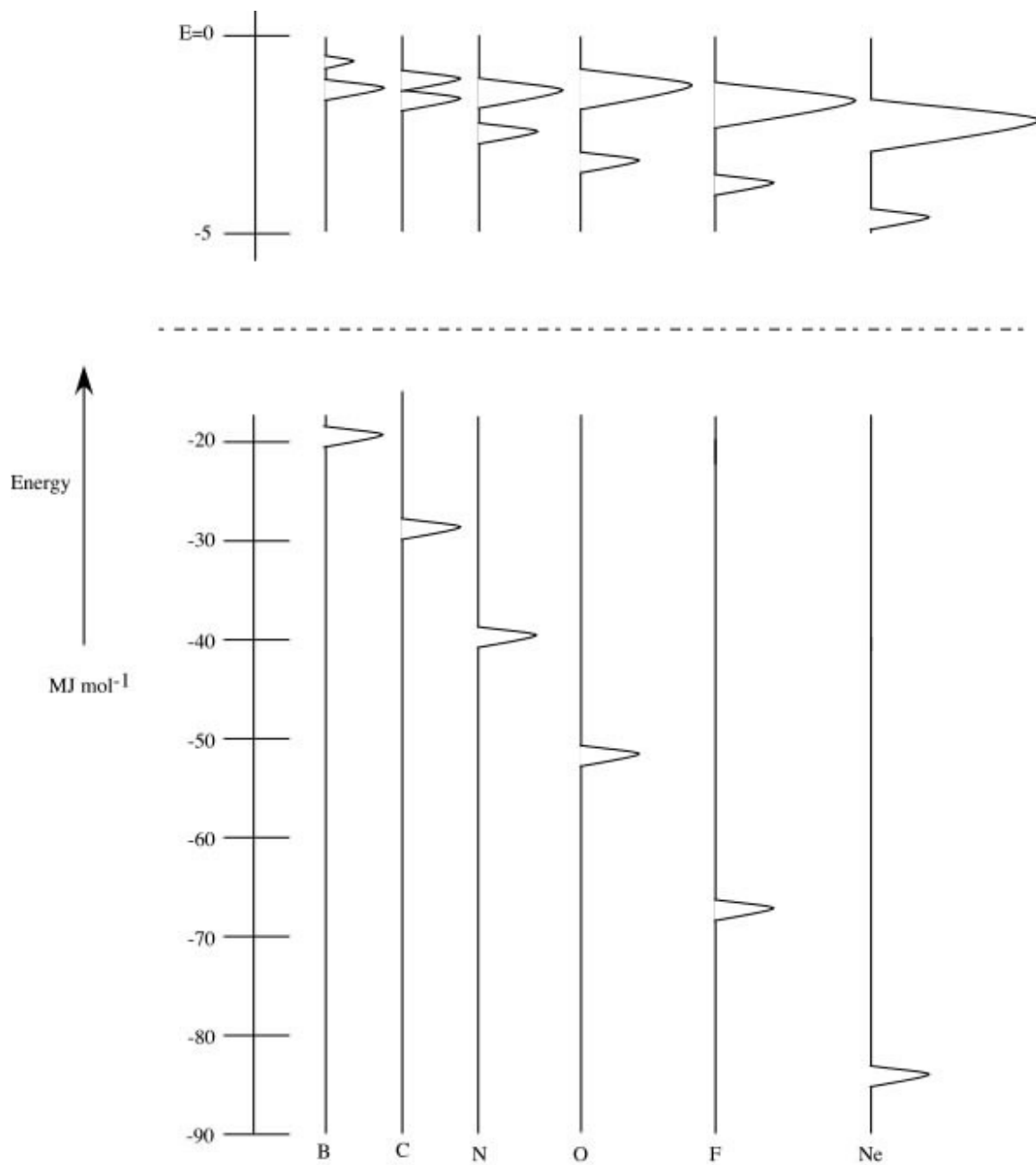


Figure V. PES for Boron (B) through Neon (Ne)

9. Answer the following questions after looking at the PES for hydrogen through neon.
- Would you agree or disagree with the following statement? Explain.
'The electrons in the second shell all have the same energy.'
 - How many 'subshells' are found in the second shell? How many 'subshells' are found in the first shell?
 - How many electrons are in each subshell in the second shell? In the first shell?
 - Moving systematically from lithium to neon;
 - How many electrons are in the first shell?
 - what happens to the energy required to remove an electron in the first shell moving from left to right in the second period? Support your observation with a meaningful explanation.
 - What happens to the energy of the electrons in the outer most shell?
10. Look at the PES for the elements in the third period (sodium – argon) and briefly describe your observations. Any surprises? Briefly explain your observations.

13. Look at the PES for potassium, calcium and scandium. Something very interesting happens when we look at the PES for scandium that has not occurred in any element prior to scandium. Briefly explain.
14. If one electron is removed from scandium, which electron (identify the shell and subshell) requires the least amount of energy to remove?

This activity along with the activity that invents shells provide experimental data for an electron configuration for elements in the periodic table.

We have not invented orbitals or electron spin.

Another experiment was performed by two researchers in 1920. Stern and Gerlach investigated the behavior of gas phase silver atom moving in a magnetic field. To interpret their experiment they had to conclude that the electron has another property besides mass and charge. What they called spin. Since the electron has charge and is 'spinning' it can produce a magnetic field. The Stern-Gerlach experiment demonstrated that electrons produce magnetic fields. The experiment suggested that there were two possible spin states for an electron. Silver has an odd number of electrons so must have an unpaired electron, and exhibits some magnetic properties. Elements with all the electrons paired are nonmagnetic.

Additional information regarding the behavior of the electron in terms of its spin has accumulated over the years.

- 1) electrons with the same spin do not like to be in the same region of space and therefore have a low probability of being close together. The region of space that electrons with opposite spin are excluded is called an orbital.
- 2) Electrons with opposite spin can occupy the same region of space.

The Pauli Exclusion Principle summarizes the behavior of electrons as it relates to spin an orbital occupancy. No more than two electrons can occupy an orbital, and the spins of these electrons must be opposite.

How can (2p subshell) six electrons distribute themselves? No more than two electrons can occupy the same region of space, and a 2p subshell can hold a maximum of six electrons then we can conclude that three unique regions of space each with two electrons. So the question is how can these three regions of space (in 3-dimensional space) arrange themselves so they have the same energy and do not impinge on each other? We find that the only arrangement is a dumb-bell shape orbital, each aligned along the axis of a 3-dimensional Cartesian coordinate system.

NOTE: The PES spectrum that will be used in this activity will have energy on the y-axis and number of electrons on the x-axis. The energies on the y-axis are negative, so the lowest (most negative) energy is on the bottom of the graph and zero energy (the electron is separated from the nucleus) is at the top of the graph.

If we generate the energies of the electrons in the atoms using PES and place energy on the y-axis we can build the energy level diagram for a multi-electron atom. Doing it this way allows us only to show the energy level diagram with energies for only those subshells that exist in the atom.

