Key

ACTIVITY 07-1

Electromagnetic Radiation

WHY?

Electromagnetic radiation, which is also called light, is an amazing phenomenon. It carries energy and has characteristics of both particles and waves. We can see only a small region of the electromagnetic spectrum, which we call *visible light*. The absorption and emission of electromagnetic radiation by atoms and molecules serve as powerful tools used to probe molecular structure and chemical reactions. They form the basis of medicine's magnetic resonance imaging and are intrinsic to many analytical techniques used to monitor the environment and manufacturing processes. Radio and television, cell phones, microwave ovens, and compact discs all utilize electromagnetic radiation.

LEARNING OBJECTIVE

- Characterize electromagnetic radiation

SUCCESS CRITERIA

- Interrelate the wavelength, frequency, momentum, and energy associated with electromagnetic radiation
- Identify the different regions of the electromagnetic spectrum

INFORMATION

During the nineteenth century, research in the areas of optics, electricity, and magnetism provided convincing evidence that electromagnetic radiation consists of two oscillating waves. One wave corresponds to an electric field, and the other wave corresponds to a magnetic field. In a vacuum, these fields oscillate perpendicular to each other and perpendicular to the direction the wave is moving. A wave is characterized by its amplitude, frequency, and wavelength. The model in this activity shows a diagram of an electromagnetic wave.

The Greek letter nu, ν, is used to represent frequency (cycles/s). Be careful to distinguish it from the English vee, v. Frequency is measured in hertz (Hz), which is expressed in cycles or oscillations per second.

The Greek letter lambda, λ, is used to represent wavelength.

During the twentieth century, scientists discovered that electromagnetic radiation also had properties normally associated with particles. This discovery led scientists to believe that electromagnetic radiation consists of particles called photons. A photon has a momentum, a specific amount of energy, and a wavelength and frequency associated with it. Thus, the properties of particles (momentum and a specific energy) and the properties of waves (wavelength and frequency) are blended together.

The wavelength and frequency of electromagnetic radiation extend essentially from 0 to infinity. The electromagnetic spectrum is viewed as split into different regions. These regions are determined by the nature of instrumentation (sources, wavelength selectors, and detectors) used in the different regions. The model in this activity also includes a chart of the electromagnetic spectrum.

MODEL: PROPERTIES OF ELECTROMAGNETIC RADIATION

Figure 1 shows an *electromagnetic wave* with the magnetic field oscillating parallel to the z-axis, the electric field oscillating parallel to the y-axis, and the wave moving along the x-axis. The x, y, and z-axes are perpendicular to each other.

The *wavelength* is the distance between any two corresponding points, e.g., from one maximum of the electric field to the next.

The *frequency* is the number of wavelengths that pass a point on the x-axis each second.

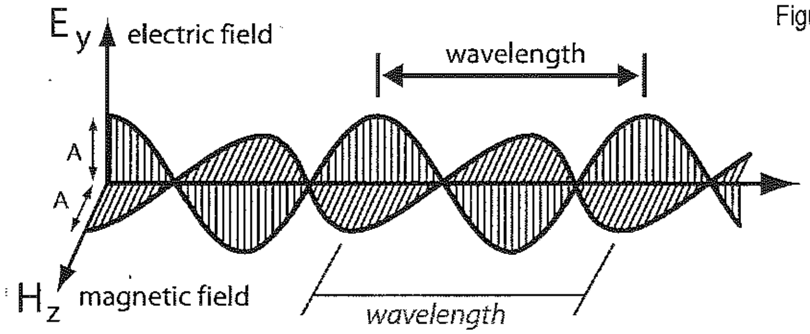


Figure 1

The chart shows the different spectral regions of the electromagnetic spectrum and indicates the approximate frequencies and wavelengths for each. The boundaries between the regions are diffuse.

Figure 2

Frequency (Hz)	Spectral Region	Wavelength (m)
10^{21}		0.3 pm
	gamma rays	
	hard x-rays	
10^{18}		0.3 nm
	soft x-rays	
	vacuum ultraviolet	
	ultraviolet	
10^{15}		300 nm
	visible	
	infrared	
	far infrared	
10^{12}		300 μm
	microwave	
10^{9}		30 cm
	radio wave	
10^{6}		300 m

Definitions

υ = frequency

λ = wavelength

p = momentum

c = speed of light
$= 2.9979 \times 10^{8}$ m/s

h = Planck's constant
$= 6.6261 \times 10^{-34}$ J s

Photon Properties

energy = $E_{photon} = h\upsilon$

momentum = $p = h / \lambda$

frequency = $\upsilon = c / \lambda$

KEY QUESTIONS

1. In the model, what is the equation showing the relationship between the energy (E) of a photon and the frequency of light (v)?

$$E = hv$$

2. What is the equation showing the relationship between the frequency (v) and wavelength (λ) of light?

$$v = \frac{c}{\lambda}$$

3. What is the equation showing the relationship between the momentum of a photon (p) and wavelength (λ)?

$$p = \frac{h}{\lambda}$$

4. If two waves are traveling at the same speed along the x-axis, will the one with the longer wavelength have the larger or smaller frequency? Explain in terms of the number of wavelengths that pass a given point on the x-axis in 1 second.

   The one with the longer wavelength will have the smaller frequency because fewer peaks will pass a given point in a given amount of time.

5. Is the energy of a photon proportional or inversely proportional to its frequency?

   The energy is directly proportional to frequency (see Key Question 1).

6. Is the momentum of a photon proportional or inversely proportional to its wavelength?

   The momentum is inversely proportional to wavelength (see Key Question 3).

7. Which region of the electromagnetic spectrum has the shortest wavelengths?

   The shortest wavelengths are in the gamma ray region.

8. Which region of the electromagnetic spectrum has photons with the lowest energy?

   The lowest energies are in the radio frequency range.

9. From what regions of the electromagnetic spectrum have you used or encountered photons? Identify the context.

   Answers will vary, e.g., radio waves, microwaves, infrared (such as lamps or night-vision cameras), visible, UV (sunscreeen, tanning lamps), x-rays (medical).

EXERCISES

1. In the model, draw a line connecting two points on the magnetic field wave that are separated by one wavelength.

   See Figure 1; label has been added.

2. The laser in a compact disc player uses light with a wavelength of 780 nm.

   a) Calculate the frequency of this light.

$$v = \frac{c}{\lambda} = \frac{(2.9979 \times 10^{8}\ m/s)}{[(780\ nm)(1 \times 10^{-9} m/nm)]}$$

$$= 3.84 \times 10^{14}\ s^{-1}$$

   b) Calculate the energy of a single photon of this light.

$$E = hv = (6.6261 \times 10^{-34} J\ s)(3.84 \times 10^{14} s^{-1}) = 2.54 \times 10^{-19} J$$

   c) Calculate the momentum of a single photon of this light.

$$p = \frac{h}{\ddot{e}} = \frac{(6.6261 \times 10^{-34} Js)}{[(780nm)x(1 \times 10^{-9} m/nm)]}$$

$$p = \frac{6.621 \times 10^{-34} J s}{780 nm \times \left(\frac{10^{-9} m}{nm}\right)} \times \frac{kg\, m^2 s^{-2}}{J}$$

$p = 8.50 \times 10^{-28}\ kg\, m/s$ *(momentum has units of mass × velocity)*

Note: $1 J = 1 kg\ m^2 s^{-2}$

3. Radiation with a wavelength of 100 nm can be used to remove electrons from atoms and molecules. Identify the region of the spectrum corresponding to this radiation.

   ultraviolet (more specifically vacuum ultraviolet)

4. Radiation emitted when excited states of nuclei decay has a frequency of approximately 10^{21} Hz. Identify the region of the spectrum corresponding to this radiation.

   gamma rays

5. Identify which uses photons with the higher energy: a microwave oven or a radio.

   Microwave oven photons have higher energy (E is proportional to v).

Research

In different regions of the electromagnetic spectrum radiation is produced and detected in different ways and has different applications. If you are familiar with these different properties and characteristics, you will be able to assess safety issues, understand the limitations and opportunities in various applications, and even identify new applications. You can find information on spectroscopy on the internet and in library books on the subject.

Each team should prepare a report to the class on one region of the electromagnetic spectrum. This report should address the following items.

- An object about the size of one wavelength of this radiation
- A laboratory source of the radiation
- A method for obtaining tunable monochromatic radiation
- A device that can detect the radiation
- The effect on a molecule when it absorbs the radiation
- Documented effects of the radiation on the human body
- How the radiation is being used in modern research

Activity 07-2

Atomic Spectroscopy and Energy Levels

Why?

The emission of light by the hydrogen atom and other atoms played a key role in helping scientists to understand the electronic structure of atoms. The light given off by atoms consists of narrow bands at specific wavelengths. The graph or other display of the light intensity as a function of wavelength is called an *emission* or *luminescence spectrum*. The spacing of the energies of the electrons in atoms can be obtained from luminescence spectra.

Learning Objective

- Understand how luminescence spectra can be related to the energy levels of electrons in atoms

Success Criteria

- Calculate the amount of energy absorbed or emitted by a hydrogen atom
- Relate luminescence bands to specific transitions between energy levels

Prerequisites

- **Activity 02-1:** *Atoms, Isotopes, and Ions*
- **Activity 07-1:** *Electromagnetic Radiation*

Information

A photon is produced when the electrons in an atom lose energy and make a transition from an upper energy level to a lower energy level.

Conservation of energy requires that the energy of the photon ($h\nu$) must equal the difference in energy between the two levels.

The model shows a luminescence spectrum of the hydrogen atom in the vacuum ultraviolet region of the electromagnetic spectrum. The intensity of the light emitted (number of photons per second) is plotted on the y-axis, and the wavelength in nm is plotted on the x-axis.

This series of bands is called the *Lyman series*, after the physicist, Theodore Lyman, who first observed them. They are produced by transitions from excited states (higher energy levels) of the hydrogen atom to the ground state (the lowest energy level).

Each energy level is labeled with an index, n, which is also called the *quantum number*. The quantum number n has integer values 1, 2, 3, etc. The energy of the hydrogen atom levels is related to the quantum number and is given by the following equation:

$E_n = -2.178 \times 10^{-18}\, Z^2 / n^2$ Joules where Z is the atomic number for hydrogen, (Z=1).

MODEL: LUMINESCENCE SPECTRUM AND ENERGY LEVELS OF THE HYDROGEN ATOM

Figure 1

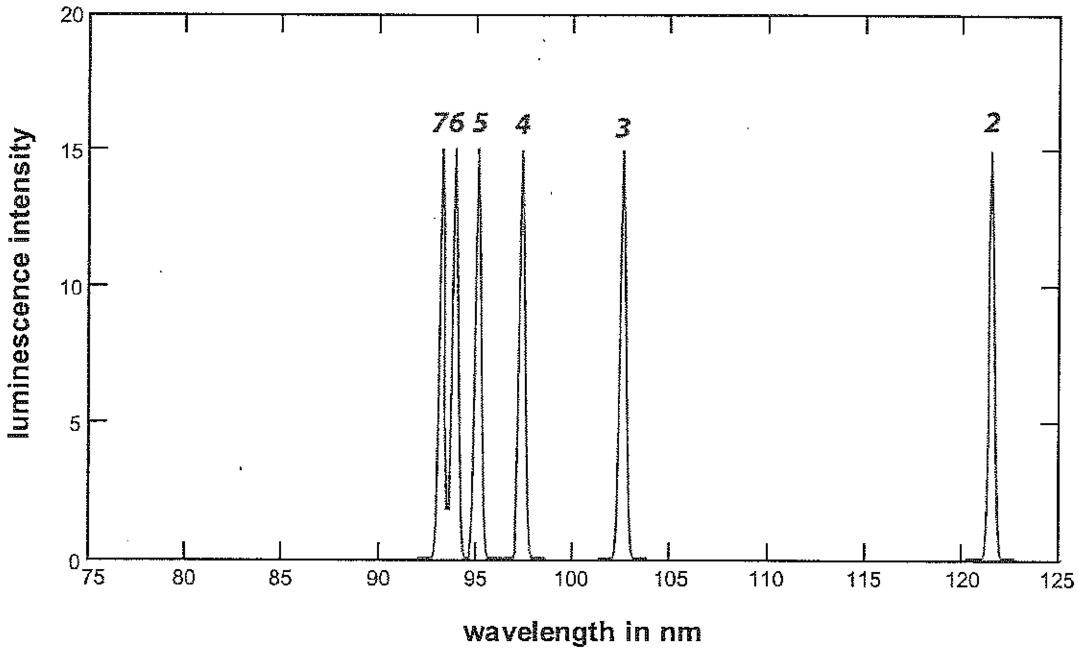
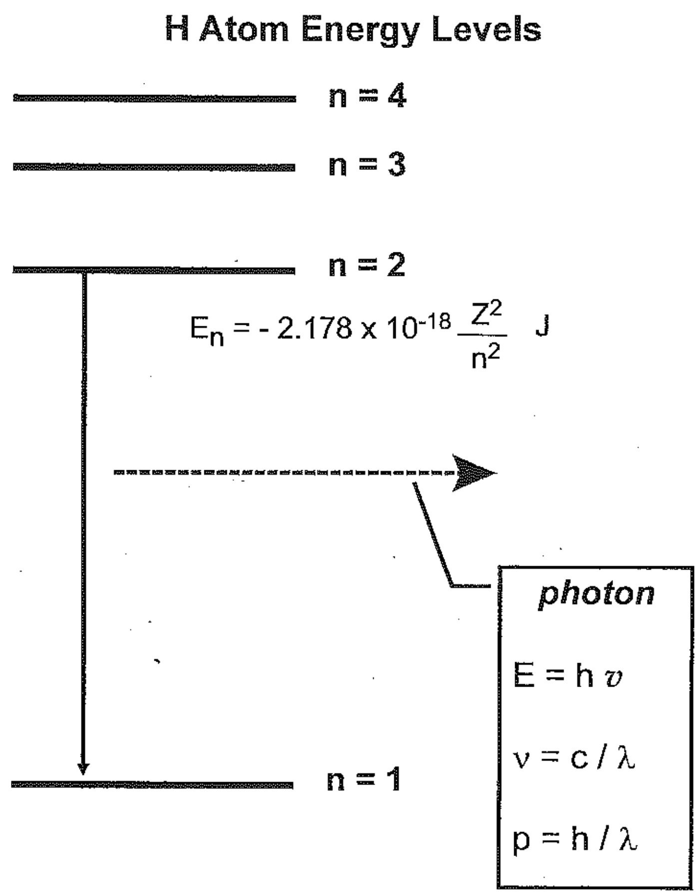


Figure 2



$$E_n = -2.178 \times 10^{-18} \frac{Z^2}{n^2} \text{ J}$$

KEY QUESTIONS

1. What is the equation that gives the possible energies (E_n) of the electron in the hydrogen atom?

$$E_n = -2.178 \times 10^{-18} \left(\frac{Z^2}{n^2} \right) J$$

2. What determines the energy of a photon that is emitted in the hydrogen atom luminescence?

   The energy difference between the final and initial levels as determined by the quantum numbers, n, for those levels using the equation in Key Question 1.

3. How can the wavelength of a photon be calculated from its energy?

   $E = h\upsilon$ and $\upsilon\lambda = c$ so substituting for υ and rearranging gives

$$\lambda = \frac{hc}{E}$$

TASKS

1. In the luminescence spectrum shown in the model, assign the lines to transitions between the hydrogen atom energy levels. To aid in this assignment, complete Table 1 below. The first two rows have been completed for you. If you are working in a team of four, each person may do one calculation.

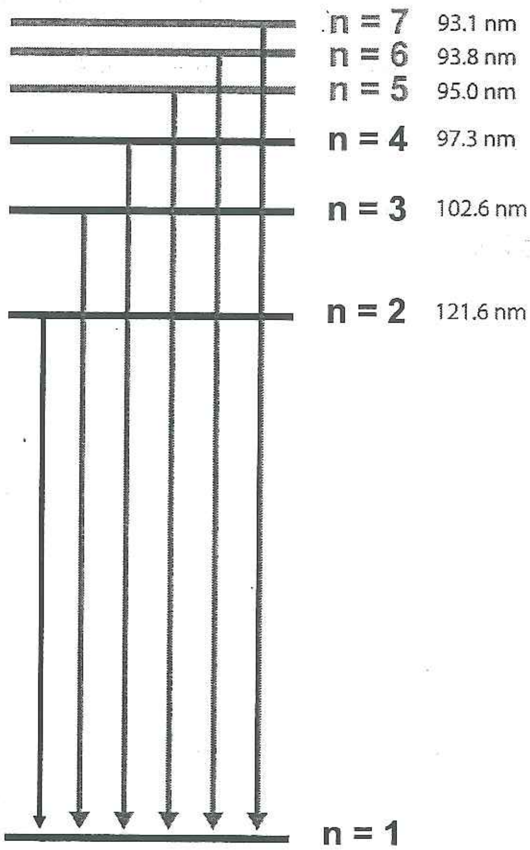
Table 1 Energies of H Atom Levels and Transitions

n (upper)	n (lower)	E(upper) in J	ΔE = E(upper) − E(lower)	λ in nm
2	1	-0.5445×10^{-18} J	1.634×10^{-18} J	121.6 nm
3	1	-0.2420×10^{-18} J	1.936×10^{-18} J	102.6 nm
4	1	-0.1361×10^{-18} J	2.042×10^{-18} J	97.3 nm
5	1	-0.0871×10^{-18} J	2.091×10^{-18} J	95.0 nm
6	1	-0.0605×10^{-18} J	2.118×10^{-18} J	93.8 nm
7	1	-0.0444×10^{-18} J	2.134×10^{-18} J	93.1 nm

2. Above each peak in the luminescence spectrum, write the quantum number of the upper level involved in the transition corresponding to that peak. Use your calculated wavelengths in Table 1 to help you make this assignment.

   See Figure 1; the quantum numbers appear above the peaks.

3. In the energy-level diagram below (which is based on Figure 2 from the model), draw arrows to represent the transitions corresponding to the spectral bands. The arrow from $n = 2$ to $n = 1$ has been done for you. Label each arrow with the wavelength of the photon produced by that transition. Add additional energy levels to the diagram as needed, and label them with their values for the quantum number n.



Got It!

1. Compare the transition that occurs when the electron in the hydrogen atom drops from energy level $n = 2$ to $n = 1$ to the transition that occurs from $n = 3$ to $n = 1$.

   a) Which transition causes the larger change in the energy of the hydrogen atom?

   3 to 1

   b) Which transition will produce light with the longer wavelength?

   2 to 1 because the energy is less, so the frequency is lower, and the wavelength is longer

2. Why doesn't the luminescence of the hydrogen atom produce light at all wavelengths?

   The energy levels are discrete not continuous, and electrons can only go from one energy level to another, and emit a photon that has an energy equal to the difference in the energies of those levels. The wavelengths observed correspond to the photon energies.

EXERCISES

1. a) What is the wavelength of light that is absorbed when an electron in the hydrogen atom goes from the energy level $n = 2$ to $n = 4$?

The energy difference can be calculated using the values from Table 1 for E(upper):

$$\Delta E = E_4 - E_2 = (-0.1361 \times 10^{-18}\ J) - (-0.5445 \times 10^{-18}\ J) = 0.4084 \times 10^{-18}\ J$$

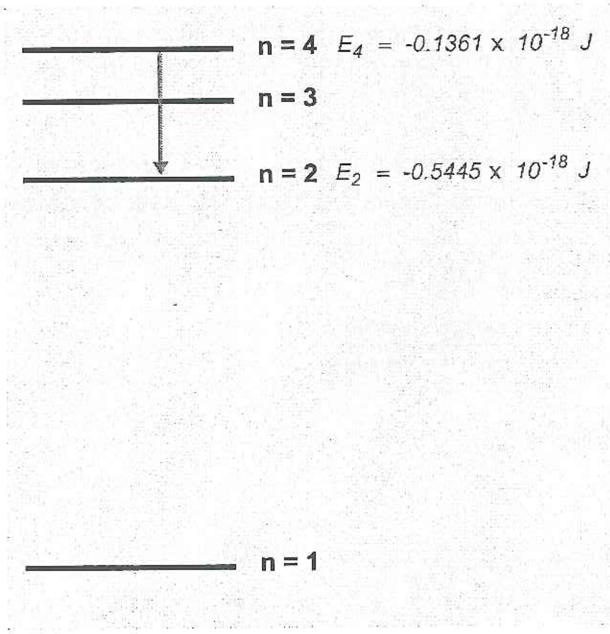
The equation from KQ 3 may then be used to calculate the wavelength:

$$\lambda = \frac{hc}{\Delta E} = \frac{(6.6261 \times 10^{-34}\ J\ s)(2.9979 \times 10^{8}\ m/s)}{0.4084 \times 10^{-18}\ J}$$
$$= 4.864 \times 10^{-7}\ m$$
$$= 486.4\ nm$$

b) In which region of the spectrum is this light?

visible

c) Illustrate this transition in an energy level diagram similar to that used in the model.



Problems

1. On Earth the ionization energy of atomic hydrogen is 1312 kJ/mol. On another planet the temperature is so high that essentially all the hydrogen atoms have the electron in the $n = 3$ quantum state. What is the ionization energy of atomic hydrogen on that planet?

   Ionization requires completely removing an electron from an atom, i.e. going from its bound (negative) energy value to a final energy of zero. Thus, the energy required to ionize a single hydrogen atom is given by the following equation after substituting $Z = 1$ and $n = 1$.

   $$E_{ionization} = 0 - \left[-2.178 \times 10^{-18} \left(\frac{Z^2}{n^2} \right) J \right]$$

   If the electron is in the $n = 3$ quantum state, then the energy is given by the same equation after substituting $Z = 1$ and $n = 3$.

   Notice that the ionization energy decreases as $1/n^2$.
   Consequently the ionization energy from $n = 3$ will be

   $$E_{ionization} = 0 - \left[-2.178 \times 10^{-18} \left(\frac{1^2}{3^2} \right) J \right] = 2.420 \times 10^{-19}\ J$$

   To express this result in kJ/mol, multiply by Avogadro's number:

   $(2.420 \times 10^{-19}\ J)(6.0221 \times 10^{23}\ mol^{-1}) = 1.457 \times 10^{5}\ J/mol = 145.7\ kJ/mol$

   Note: students may also be encouraged to recognize that the ionization energy stated in the problem for $n = 1$ comes from multiplying the Rydberg constant (2.178×10^{-18} J) by Avogadro's number, and that the ionization energy they have calculated is just $1/n^2 = 1/9$ of the stated ionization energy for $n = 1$.

2. Microwaves are used to heat food in microwave ovens. The microwave radiation is absorbed by moisture in the food. This absorption heats the water, and as it becomes hot so does the rest of the food. How many photons having a wavelength of 3.00 cm would have to be absorbed by 1.00 g of water to raise its temperature by 1.00 °C?

   $$\text{number of photons} = \frac{\text{energy needed}}{\text{energy of one photon}}$$

   energy of one photon

   $$E = \frac{hc}{\lambda}$$

   $$E = \frac{(6.6261 \times 10^{-34}\ J\ sec)(2.9979 \times 10^{8}\ m/sec)}{(3.00\ cm)\left(\frac{1\ m}{100\ cm}\right)}$$

   $$= 6.621 \times 10^{-24}\ J/photon$$

   The energy needed to raise 1.00 g of water by 1.00°C = 4.184 J

   Divide this energy by the energy of one photon

   $$\frac{4.184\ J}{6.621 \times 10^{-24}\ J/photon} = 6.32 \times 10^{23}\ photons$$

   Look at that! It takes about a mole of microwave photons to raise the temperature of 1 g of water by 1 degree.

Activity 07-3

The Description of Electrons in Atoms

Why?

A description of electrons in atoms includes their energies and a quantitative picture of how they are distributed in space. This description is needed to understand how molecules are formed from atoms, how to synthesize new molecules, and how molecules function, i.e., the relationship between their structure, their reactivity, and their function in medicines, biological systems, and technological devices.

Learning Objective

- Gain an understanding of atomic orbitals

Success Criteria

- Correctly identify particular types of atomic orbitals
- Interrelate characteristics of atomic orbitals such as their name, shape, orientation in space, nodal pattern, extension in space, and energy

Prerequisite

- **Activity 07-2:** *Atomic Spectroscopy and Energy Levels*

Information

Realizing that light waves have momentum, and knowing that momentum is a property of particles, de Broglie proposed that particles, like electrons, must correspondingly have properties of waves. Experiments proved this to be true.

This success led Schrödinger to invent a mathematical equation that could be solved to provide wave functions describing electrons. This equation is now very famous and is called the Schrödinger equation.

While the Schrödinger equation is too complicated to be solved exactly for atoms with more than one electron, it can be solved exactly for atoms or ions with a single electron, like the hydrogen atom. The wave functions for the hydrogen atom are used to provide approximate wave functions for all other atoms. These approximate one-electron wave functions are called *atomic orbitals*.

While an atomic orbital is a mathematical function describing a single electron, chemists often think of the orbital as the region of space in which an electron can be found. An orbital can be represented by drawing a boundary surface to identify that the electron has a 90% probability of being within that surface. Such boundary surfaces for some atomic orbitals are shown in the model.

While the energy levels of the hydrogen atom and ions with only one electron are determined by a single index or quantum number, $\boldsymbol{n}$, Schrödinger discovered that more quantum numbers are involved in determining the energies, shapes, and orientations of the atomic orbitals. In addition to $\boldsymbol{n}$, the quantum numbers ℓ and $\boldsymbol{m_\ell}$ are also needed. These quantum numbers are called the *principal quantum number* ($\boldsymbol{n}$), the *angular momentum* or *azimuthal quantum number* (ℓ), and the *magnetic quantum number* ($\boldsymbol{m_\ell}$).

MODEL: ATOMIC ORBITALS (WAVE FUNCTIONS) FOR ONE-ELECTRON ATOMS

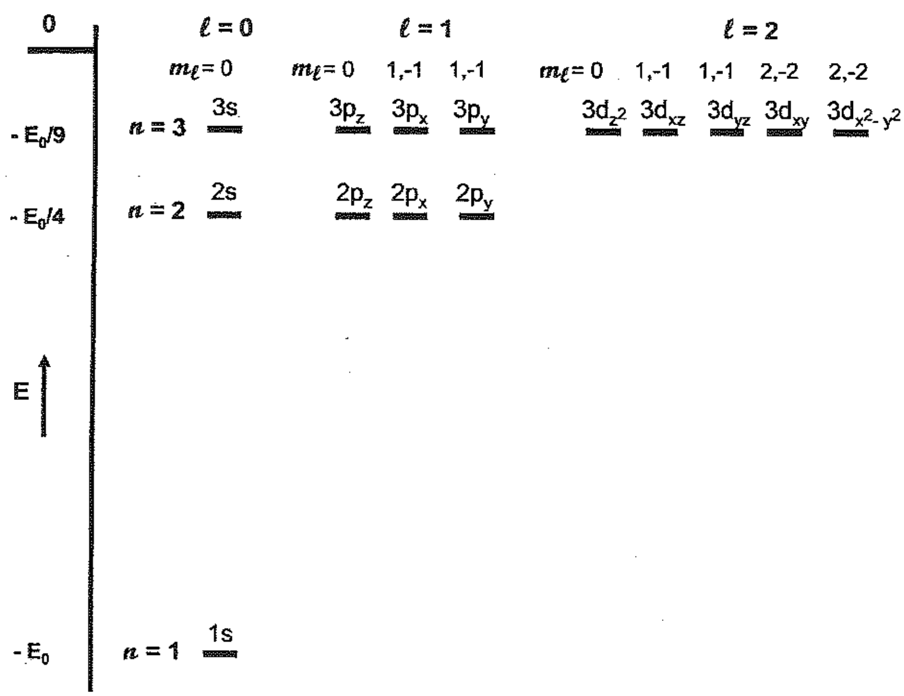
Table 1

Quantum Numbers

Name	Characterizes	Symbol	Allowed Values
Principal	size energy total nodes = $n-1$	n	n = 1, 2, 3, ... to infinity
Angular Momentum or Azimuthal	shape energy in multi-electron atoms planar nodes = ℓ	ℓ	$\ell = 0, 1, 2, \ldots n - 1$
Magnetic	orientation	m_ℓ	$m_\ell = -\ell, -\ell+1, \ldots 0, \ldots \ell-1, \ell$ $2\ell + 1$ values

Figure 1

Energy Levels and Orbital Labels



For atoms or ions with only 1 electron, orbital energies are ordered as follows:

1s < 2s=2p < 3s=3p=3d < 4s=4p=4d=4f < 5s=5p=5d=5f < 6s=6p=6d < 7s

For multi-electron atoms, orbital energies increase in the following order:

1s<2s<2p<3s<3p<4s<3d<4p<5s<4d<5p<6s<4f<5d<6p<7s<5f<6d

MODEL: ATOMIC ORBITALS (WAVE FUNCTIONS) FOR ONE-ELECTRON ATOMS (CONTINUED)

Figure 2

Shapes and Sizes of Atomic Orbitals

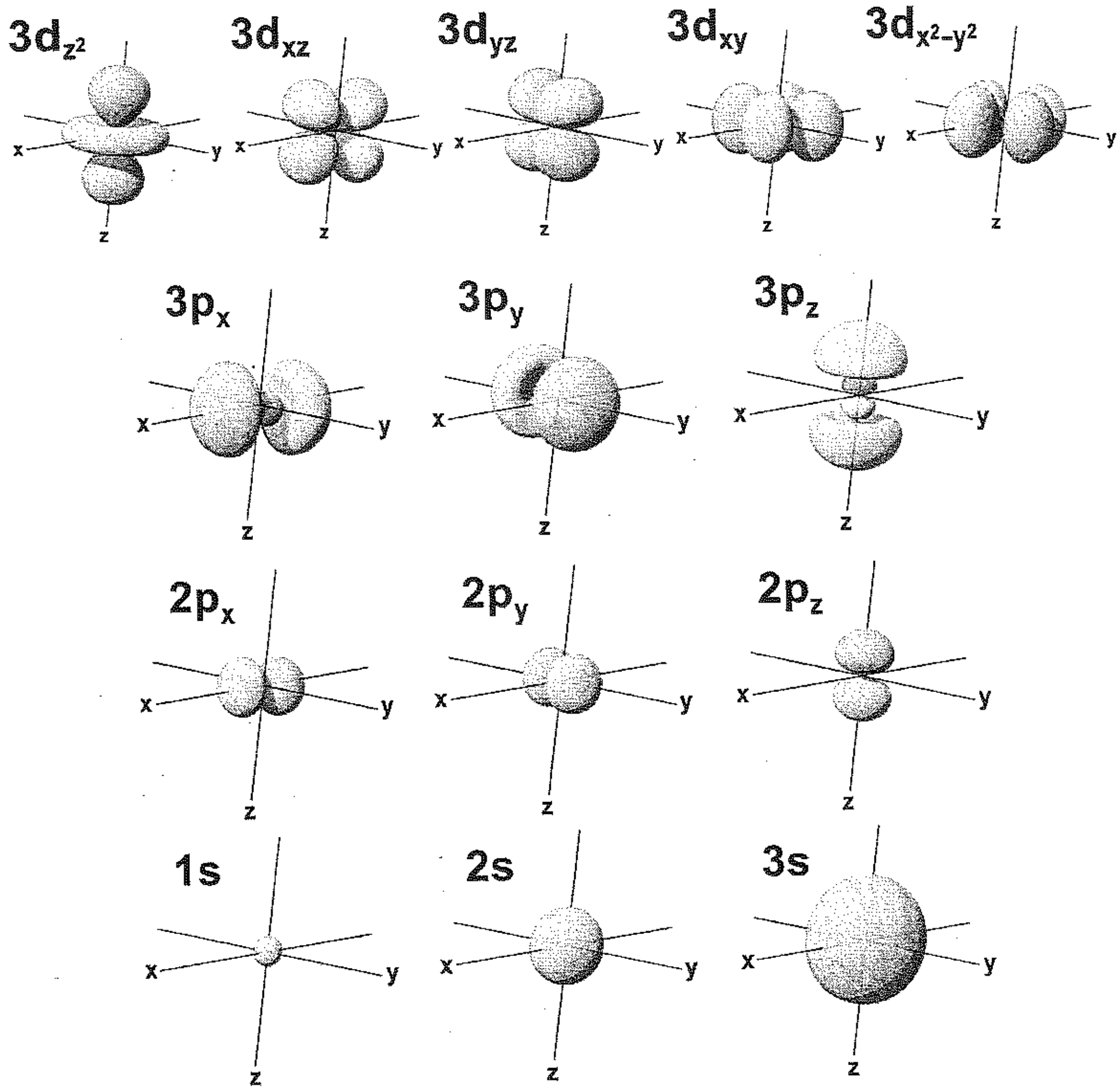
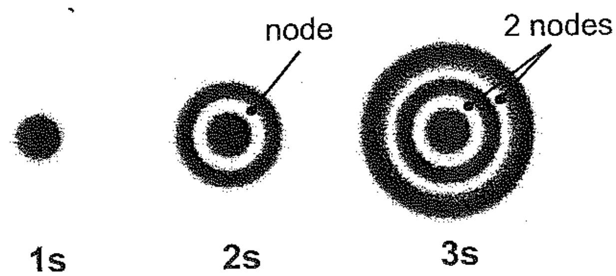


Figure 3

Radial Nodes in S-Orbitals



KEY QUESTIONS

1. What are the characteristic shapes of s, p, and d orbitals that distinguish them from each other?

   s orbitals look like spheres

   p orbitals look like two balloons tied together

   d orbitals look like four balloons tied together, except one orbital looks like two balloons surrounded by a ring

2. Which quantum number identifies the shape of an orbital?

   the ℓ (el) or angular momentum quantum number

3. What happens to the size of a particular type of orbital, as the principal quantum number increases? Consider s orbitals, for example.

   The orbitals increase in size.

4. Which quantum numbers determine the energy of an orbital in an atom with more than one electron?

   the n and ℓ quantum numbers

5. For each value of n = 1, 2, and 3, what are the possible values for ℓ, and what are the labels for the orbitals with these ℓ values? (For example s, p, or d.)

n	possible ℓ values	orbital labels
1	*0*	*1s*
2	*0 and 1*	*2s and 2p*
3	*0, 1 and 2*	*3s, 3p and 3d*

6. For each value of ℓ = 0, 1, and 2, what are the possible values for m_ℓ, and what are the labels, written as subscripts, for the orbitals with these m_ℓ values?

ℓ	possible m_ℓ values	orbital labels
0	*0*	*s*
1	*-1, 0, 1*	p_x p_y p_z
2	*-2, -1, 0, 1, 2*	d_{xy} d_{yz} d_{xz} $d_{x^2-y^2}$ d_{z^2}

7. Which orbitals in the model have a plane that includes the origin where the probability of finding the electron is zero? The *origin* is where the axes cross. These planes are called *angular nodal planes*. A *node* is the place where a wave has zero amplitude.

   p and d orbitals in the model – actually all orbitals except s

8. What is the relationship between the value of the azimuthal quantum number and the number of angular nodal planes?

   They are equal.

9. In addition to angular nodal planes, there are *radial nodes*. These nodes occur for all angles at some distance from the nucleus. Which orbitals in the model have radial nodes? Carefully compare the 2p and 3p orbitals before you answer this question.

Radial nodes are shown for 2s and 3s orbitals, and if you look carefully also for 3p.

EXERCISES

1. The total number of nodes in an orbital is equal to n–1. This number is split between radial nodes and angular nodal planes. Show that your answers to Key Questions 7 and 9 are consistent with this fact.

n = 1, no nodes

n = 2, one node total: one radial node in the s orbital and one angular node in the p orbital.

n = 3, two nodes total: two radial nodes in the s orbital, one angular node and one radial node in the p orbital, and two angular nodes in the d orbitals (but it looks like the $3d_{z^2}$ orbital is an exception, however this orbital can also be represented by two other orbitals, each of which has two angular nodes).

2. For n = 4, identify the possible values for ℓ.

0, 1, 2, 3

3. For ℓ = 3, identify the possible values for m_ℓ.

-3, -2, -1, 0, 1, 2, 3

4. Identify the number of angular nodes in an ℓ = 3 orbital.

Three, following the pattern of ℓ=0 (none), ℓ=1 (one), and ℓ=2 (two) so ℓ=3 must have 3.

5. Identify the following for the 1s, 2s, and 3s orbitals:

a) total number of nodes

For 1s, 0, for 2s, 1 and for 3s, 2.

b) number of angular nodes and the number of radial nodes

For 1s, 0 angular and 0 radial

For 2s, 0 angular and 1 radial

For 3s, 0 angular and 2 radial

6. Identify the relationship between the total number of nodes and the energy of the orbital.

The greater the number of nodes, the higher the energy.

7. Identify the total number of nodes, the number of angular nodes, and the number of radial nodes for a 2p orbital.

A 2p orbital has 1 angular node and 0 radial nodes for a total of 1 node.

8. Identify the total number of nodes, the number of angular nodes, and the number of radial nodes for a 3p orbital.

A 3p orbital has 1 angular node and 1 radial node for a total of 2 nodes.

9. Identify the total number of nodes, the number of angular nodes, and the number of radial nodes for a 3d orbital.

A 3d orbital has 2 angular nodes and 0 radial nodes for a total of 2 nodes.

10. Based on what you have learned so far about atomic orbitals, determine the total number of orbitals with $n = 4$

For $n = 4$

$\ell = 0$, 4s   1 orbital

$\ell = 1$, $4p_x$ $4p_y$ $4p_z$ 3 orbitals

$\ell = 2$, $4d_{xy}$ $4d_{yz}$ $4d_{xz}$ $4d_{x2-y2}$ $4d_{z2}$ 5 orbitals

$\ell = 3$, m_ℓ goes from – 3 to + 3 so there must be 7 orbitals, called f-orbitals.

So for $n = 4$, there are 16 orbitals total.

ACTIVITY 07-4

Multi-electron Atoms, the Aufbau Principle, and the Periodic Table

WHY?

To construct the other elements from the simplest element, hydrogen, protons and neutrons are added to the nucleus and electrons are added to the orbitals in order of increasing energy. This is called the building-up principle (*aufbau* in German). By knowing the orbital energy-level structure and the number of electrons in an element, you can determine the electron configuration and thus the properties of the element. This information is summarized in the *Periodic Table of the Elements*, which you can use as a tool to identify materials with similar or contrasting chemical and physical properties.

LEARNING OBJECTIVE

- Master the procedure for determining the electronic configuration of atoms and ions

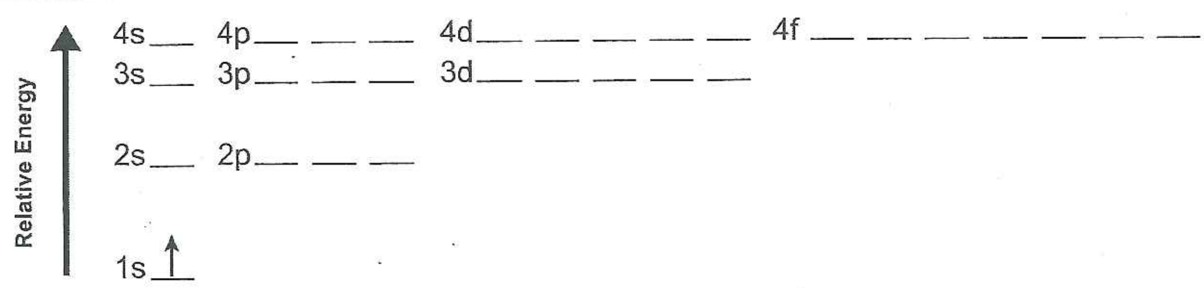
SUCCESS CRITERIA

- Correctly write the electron configuration of atoms and ions
- Relate electron configuration to positioning in the Periodic Table

PREREQUISITES

- **Activity 07-2:** *Atomic Spectroscopy and Energy Levels*
- **Activity 07-3:** *The Description of Electrons in Atoms*

MODEL 1: ENERGY LEVEL DIAGRAM FOR THE HYDROGEN ATOM



The electron configuration **$1s^1$** is a shorthand way to describe the electron in the hydrogen atom, which is represented by an arrow.

Suggestions contributed by Vicky Minderhout and colleagues at Seattle University

Key Questions

1. In writing the electron configuration for hydrogen as $1s^1$,

   a) What does the first 1 refer to?

   The first 1 refers to the principal quantum number for the orbital.

   b) What does the s refer to?

   The s refers to the type of orbital, related to the shape and/or the angular momentum quantum number.

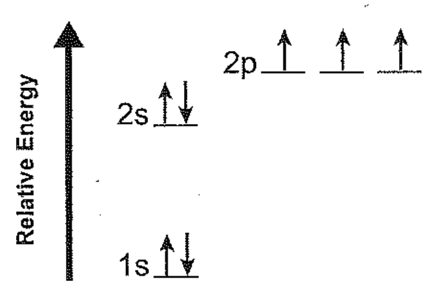
   c) What does the superscript 1 refer to?

   The superscript 1 refers to the number of electrons in the orbital.

2. Why are there different numbers of lines drawn after the symbols, e.g., 4s has one line, 4p has 3 lines, 4d has 5 lines and 4f has seven lines?

   The numbers of lines indicate the number of orbitals of the same type (having the same angular momentum quantum number): one s orbital, three p orbitals, five d orbitals, and seven f orbitals.

Model 2: Energy Level Diagram for the Nitrogen Atom



The electron configuration for the nitrogen atom is $\mathbf{1s^22s^22p^3}$. The up and down arrows represent two different spin angular momentum states of the electron.

Key Questions

3. What happens to the energies of the 2s and 2p orbitals when the atom has more than one electron?

   The p orbitals have a greater relative energy than the s orbitals in the nitrogen atom. In the hydrogen atom, the energies of the 2s and the 2p orbitals are the same (as illustrated in Model 1).

4. In the notation $2p^3$, what information is provided by the 2, the p, and the 3?

   The number 2 is the principal quantum number of the orbital. The p describes the type of orbital. The 3 tells the total number of electrons in the p orbitals.

5. What information about the electron is provided by the direction of the arrow in the diagram?

The arrows describe the spin of the electrons. Arrows pointing in opposite directions describe electrons of opposite spins.

6. Are two electrons with the same spin angular momentum described by the same atomic orbital in nitrogen? Explain your answer.

No, two electrons with the same spin occupy different orbitals. This is illustrated in Model 2. Nitrogen has three electrons in three different 2p orbitals. Each of these electrons has the same spin, but any orbital with two electrons has the electrons with opposite spins.

7. If two atomic orbitals have the same energy, will the electrons pair up in one of them or go into different orbitals?

According to Model 2, electrons occupy different orbitals with the same energy rather than pairing up in the same orbital whenever possible. Atomic orbitals with the same energy are singly occupied by electrons with the same spin. We can infer from this model that electrons with the same spin cannot occupy the same orbital.

8. Explain why the three 2p electrons in nitrogen have the configuration $2p_x^1 2p_y^1 2p_z^1$ and not $2p_x^3$ or $2p_x^2 2p_y^1$.

The three 2p electrons in nitrogen cannot have the configuration $2p_x^3$ *because the Model shows that only two electrons can occupy an orbital, not three. The three 2p electrons in nitrogen do not have the configuration* $2p_x^2 2p_y^1$ *because, according to Model 2, electrons fill equally energetic orbitals singly before pairing up. This makes sense because electrons occupying the same orbital would experience stronger electrical repulsion than electrons in different orbitals.*

Information

All atoms have the same kinds of orbitals as the hydrogen atom, but the energies of these orbitals change as the number of protons and number of electrons of the atom changes. The following guidelines are used to identify the orbitals that are occupied by electrons in any atom. These guidelines are derived from quantum mechanics and the solutions to Schrödinger's equation.

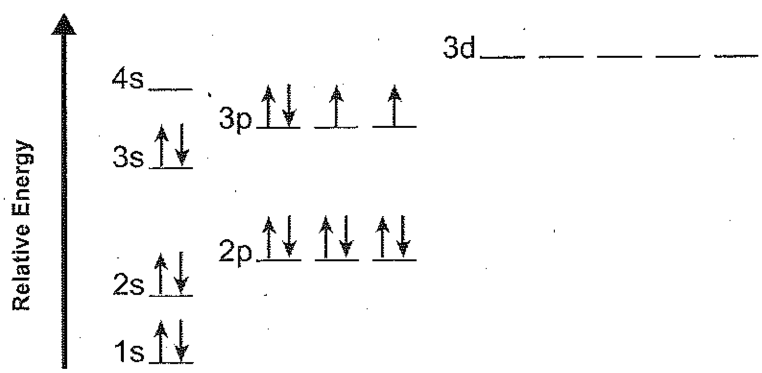
The *Aufbau Principle* says that, as protons are added to the nucleus to build up the elements, electrons are added first to the lowest energy atomic orbitals available before they fill higher energy orbitals. The name derives from *aufbau* in German, which means *building-up*. The Aufbau Principle makes sense because it produces the lowest energy or most stable arrangement of the electrons in the atom.

The *Pauli Exclusion Principle* says that two electrons cannot have the same set of quantum numbers simultaneously. This principle determines the number of electrons that can occupy each orbital. In addition to the three quantum numbers introduced in *Activity 07-3: The Description of Electrons in Atoms*, there is a fourth quantum number that is attributed to electron angular momentum. Electron spin angular momentum is a property that is described by Dirac's relativistic formulation of quantum mechanics. In some ways it is similar to a basketball or tennis ball spinning, yet there are important differences. Electron spin angular momentum is best regarded as the intrinsic angular momentum carried by an electron and not as the electron actually spinning. Dirac showed that each electron can have two values for the spin angular momentum quantum number, m_S: +½ and –½. So two electrons can be in each orbital and have the same values for n, ℓ, and m_ℓ because they have different values for m_S. The two different spin angular momentum states for electrons are represented in orbital diagrams by up and down arrows or by the values +½ and –½ for the spin quantum number, m_S.

Hund's Rule says that if multiple orbitals with the same energy are available, then the unoccupied orbitals will be filled by electrons with the same spin before electrons with different spins pair up in occupied orbitals. Hund's Rule makes sense because electrons repel each other. If they are in the same orbital, they will be close together and their energy will be higher than it would be if they were separated in different orbitals.

EXERCISES

1. Complete the energy level diagram below and write the electron configuration for sulfur.



The electron configuration for sulfur is $1s^2 2s^2 2p^6 3s^2 3p^4$.

2. In your energy level diagram for sulfur, above, identify features that illustrate

   a) the Aufbau Principle

   Placing the 16 electrons in the lowest energy levels possible is an illustration of the Aufbau Principle.

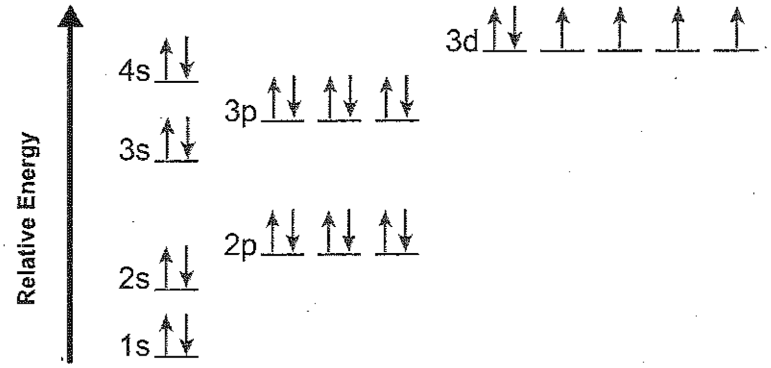
   b) the Pauli Exclusion Principle

   Placing no more than two electrons in an orbital illustrates the Pauli Exclusion Principle.

c) Hund's Rule.

Hund's Rule states that electrons occupy orbitals singly before pairing up. There are four electrons in the three 3p orbitals. Two of the electrons have paired up but the other two electrons occupy the remaining p orbitals singly.

3. Complete the energy level diagram below and write the electron configuration for iron.



The electron configuration for iron is $1s^22s^22p^63s^23p^64s^23d^6$.

MODEL 3: THE PERIODIC TABLE OF ELEMENTS

The Periodic Table of the Elements

Key: 1.008 — Mean atomic mass (amu) / Molar Mass (g/mol); H — Symbol; Hydrogen — Name; 1 — Atomic number

	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1.008 H Hydrogen 1																	4.00 He Helium 2
2	6.94 Li Lithium 3	9.01 Be Beryllium 4											10.81 B Boron 5	12.01 C Carbon 6	14.01 N Nitrogen 7	16.00 O Oxygen 8	19.00 F Fluorine 9	20.18 Ne Neon 10
3	22.99 Na Sodium 11	24.31 Mg Magnesium 12											26.98 Al Aluminum 13	28.09 Si Silicon 14	30.97 P Phosphorus 15	32.07 S Sulfur 16	35.45 Cl Chlorine 17	39.95 Ar Argon 18
4	39.10 K Potassium 19	40.08 Ca Calcium 20	44.96 Sc Scandium 21	47.88 Ti Titanium 22	50.94 V Vanadium 23	52.00 Cr Chromium 24	54.94 Mn Manganese 25	55.85 Fe Iron 26	58.93 Co Cobalt 27	58.69 Ni Nickel 28	63.55 Cu Copper 29	65.39 Zn Zinc 30	69.72 Ga Gallium 31	72.61 Ge Germanium 32	74.92 As Arsenic 33	78.96 Se Selenium 34	79.90 Br Bromine 35	83.80 Kr Krypton 36
5	85.47 Rb Rubidium 37	87.62 Sr Strontium 38	88.91 Y Yttrium 39	91.22 Zr Zirconium 40	92.91 Nb Niobium 41	95.94 Mo Molybdenum 42	(97.9) Tc Technetium 43	101.07 Ru Ruthenium 44	102.91 Rh Rhodium 45	106.42 Pd Palladium 46	107.87 Ag Silver 47	112.41 Cd Cadmium 48	114.82 In Indium 49	118.71 Sn Tin 50	121.76 Sb Antimony 51	127.60 Te Tellurium 52	126.90 I Iodine 53	131.29 Xe Xenon 54
6	132.91 Cs Caesium 55	137.33 Ba Barium 56	138.91 La Lathanum 57	178.49 Hf Hafnium 72	180.95 Ta Tantalum 73	183.85 W Tungsten 74	186.21 Re Rhenium 75	190.2 Os Osmium 76	192.22 Ir Iridium 77	195.08 Pt Platinum 78	196.97 Au Gold 79	200.59 Hg Mercury 80	204.38 Tl Thallium 81	207.2 Pb Lead 82	208.98 Bi Bismuth 83	(209) Po Polonium 84	(210) At Astatine 85	(222) Rn Radon 86
7	(223.02) Fr Francium 87	(226.03) Ra Radium 88	(227.03) Ac Actinium 89	(261) Rf Rutherfordium 104	(262) Db Dubnium 105	(263) Sg Seaborgium 106	(262) Bh Bohrium 107	(265) Hs Hassium 108	(266) Mt Meitnerium 109	(271) Ds Darmstadtium 110	(280) Rg Roentgenium 111	(285) Not Yet Officially Named 112						
	Alkali Metals	Alkaline Earth Metals	Transition Metals														Halogens	Noble Gases

Lathanides	140.12 Ce Cerium 58	140.91 Pr Praseodymium 59	144.24 Nd Neodymium 60	(145) Pm Promethium 61	150.36 Sm Samarium 62	152.97 Eu Europium 63	157.25 Gd Gadolinium 64	158.93 Tb Terbium 65	162.50 Dy Dysprosium 66	164.93 Ho Holmium 67	167.26 Er Erbium 68	168.93 Tm Thulium 69	173.04 Yb Ytterbium 70	174.97 Lu Lutetium 71
Actinides	232.04 Th Thorium 90	(231.04) Pa Protactinium 91	238.03 U Uranium 92	(237.05) Np Neptunium 93	(240) Pu Plutonium 94	(243.06) Am Americium 95	(247) Cm Curium 96	(248) Bk Berkelium 97	(251) Cf Californium 98	(252.08) Es Einsteinium 99	(257.10) Fm Fermium 100	(257) Md Mendelevium 101	(259.10) No Nobelium 102	(262.11) Lr Lawrencium 103

Non-Metals
Metals
Semi-Metals

Model 3: The Periodic Table of Elements (continued)

Electron Configurations

Table 1

Element	Number of Electrons	Electron Configuration
He	2	$1s^2$
Li	3	$1s^2 2s^1$
Be	4	$1s^2 2s^2$
B	5	$1s^2 2s^2 2p^1$
Ne	10	$1s^2 2s2^2 p^6$
Na	11	$[Ne]3s^1$
Al	13	$[Ne]3s^2 3p^1$
Ar	18	$[Ne]3s^2 3p^6$

Element	Number of Electrons	Electron Configuration
K	19	$[Ar]4s^1$
Sc	21	$[Ar]4s^2 3d^1$
Ti	22	$[Ar]4s^2 3d^2$
Zn	30	$[Ar]4s^2 3d^{10}$
Ga	31	$[Ar]4s^2 3d^{10} 4p^1$
Kr	36	$[Ar]4s^2 3d^{10} 4p^6$
Rb	37	$[Kr]5s^1$

Key Questions

The rows in the Periodic Table are called periods, the columns are called groups, and the elements can be grouped together in blocks. All of this structure is due to and reflects the electron configurations of the atoms. The information in the Electron Configuration Table in **Model 3** (Table 1) and the following questions should help you deepen your understanding of the Periodic Table.

9. In terms of electron configurations, why are there only two elements in Period 1?

   There are only two elements in Period 1 because the atoms of these two elements (hydrogen and helium) have one and two electrons respectively. These electrons occupy the 1s orbital. There is only one 1s orbital and this orbital can hold a maximum of two electrons.

10. In terms of electron configurations, why do Periods 2 and 3 each contain eight elements?

    The electrons of the elements in Periods 2 and 3 occupy both s and p orbitals with the principal quantum number corresponding to the period. The s orbitals can hold two electrons and the p orbitals can hold six electrons for a total of eight electrons with the same principal quantum number.

11. In terms of electron configurations, why are there 18 elements in Period 4?

In addition to the eight available spaces in the 4s and 4p orbitals, this period also includes elements where electrons fill the ten available spaces in the five 3d orbitals. Since the 3d orbitals are higher in energy than the 4s orbitals (as shown in the diagram in Exercise 3) but lower in energy than the 4p orbitals, these elements belong in the fourth Period between elements that correspond to filling the 4s and 4p orbitals. The additional ten electrons in d orbitals increase the total number of elements in Period 4 to 18.

12. A block is formed by all the elements in Groups 1 and 2. What do these elements have in common?

All of these elements have their highest energy electrons in s orbitals.

13. A block is formed by all the elements in Groups 3 through 12. What do these elements have in common?

All of these elements have their highest energy electrons in d orbitals.

14. A block is formed by all the elements in Groups 13 through 18. What do these elements have in common?

All of these elements have their highest energy electrons in p orbitals.

15. A block is formed by the 28 elements set off at the bottom of the table. What do these elements have in common?

All of these elements have their highest energy electrons in f orbitals.

16. Why are the chemical properties of Na, K, and Rb similar?

Na, K and Rb all have a single electron in an s orbital. These elements lose a single electron easily to become cations with a +1 charge. Losing the single electron in the s orbital results in a cation with a completely filled orbital.

17. In terms of their electron configurations, why do you think the elements in Group 18 are very stable, inert, and unreactive?

Group 18 elements are the noble gases. They are unreactive because their orbitals are completely filled and it would not be easy for these elements to gain or lose electrons in a chemical reaction.

18. What do the elements in each group have in common?

The elements in each group have the same ending electron configuration, although the principal quantum number will be different. For example, Table 1 shows that both Li and Na have one electron in an s orbital in the highest energy level, 2s for Li and 3s for Na. The elements in each group have the same outer electron configuration and consequently the same chemical properties.

Exercises

4. Identify three elements not in Groups 1 or 18 that you expect to have similar chemical properties. Explain why.

   Be, Mg, and Ca would be expected to have similar chemical properties because their electron configurations end in $2s^2$, $3s^2$ and $4s^2$, respectively. Loss of these outer shell electrons results in the production of cations with noble gas electron configurations. [Students may identify other groups with different chemical properties. The instructor may wish to help students distinguish between particularly good examples (such as Groups 16 and 17) and examples where group trends are weaker (such as Groups 13 through15 and some of the transition metal groups).]

5. Identify the element with the following electron configuration: $[Xe]6s^24f^{14}5d^{10}$.

   The element with this electron configuration is mercury (Hg).

6. Write the electron configuration for each of the following atoms or ions.

O	$1s^22s^22p^4$
Mg	$1s^22s^22p^63s^2$
Mg^{2+}	$1s^22s^22p^6$
Cl	$1s^22s^22p^63s^23p^5$
Cl^-	$1s^22s^22p^63s^23p^6$
N^{3-}	$1s^22s^22p^6$

Activity 07-5

Periodic Trends in Atomic Properties

Why?

Many properties of atoms have a repeating pattern when plotted with respect to atomic number. The similarities are due to the repeating pattern of electron configurations involving s, p, d, and f orbitals. These experimentally observed periodic trends actually provide evidence for the orbital and shell structure of atoms as well as the meaningful arrangement of elements in the Periodic Table. Your ability to recognize the properties of the elements from their positions in the Periodic Table will prove useful in handling chemical compounds safely, developing new materials, finding new applications of known materials, or using chemistry in medical applications.

Learning Objective

- Develop relationships between position in the Periodic Table, electron configurations, atomic radius, ionization energy, and electron affinity

Success Criteria

- Use electron configurations and position in the Periodic Table to account for the relative sizes, ionization energies, and electron affinities of different atoms
- Order elements by atomic radius, ionization energy, and electron affinity

Prerequisites

- **Activity 07-3:** *The Description of Electrons in Atoms*
- **Activity 07-4:** *Multi-electron Atoms, the Aufbau Principle, and the Periodic Table*

Information

Properties such as the size of an atom (atomic radius), the energy required to remove an electron from an atom (ionization energy), and the energy required to remove an electron from a negative atomic ion (electron affinity) can be understood in terms of the electron configuration of the atom and the balance between *electron-nucleus attraction* and *electron-electron repulsion*. An electron in an atom is attracted by the positively charged nucleus and repelled by the other electrons. How they balance depends on how effective the electrons are in getting close to each other or close to the nucleus. If the electron-nucleus attraction (e-n) has a large effect, then the atom is small, has a high ionization energy, and large electron affinity. If the electron-electron repulsion (e-e) has a large effect, then the atom is large, the ionization energy is small, and the electron affinity is very small or zero. Table 1 summarizes what happens in the progression from one atom to the next in the Periodic Table; both the nuclear charge and the number of electrons increase by 1 unit.

Table 1 Effects of Attractive and Repulsive Interactions

Interaction	Atomic Size	Ionization Energy	Electron Affinity
e-n attraction > e-e repulsion	Decreases	Increases	Increases
e-n attraction < e-e repulsion	Increases	Decreases	Decreases

Model 1: Review of Electron Configurations of Atoms

The electron configuration of an atom specifies the number of electrons in each atomic orbital.

Example: The Electron Configuration of Carbon

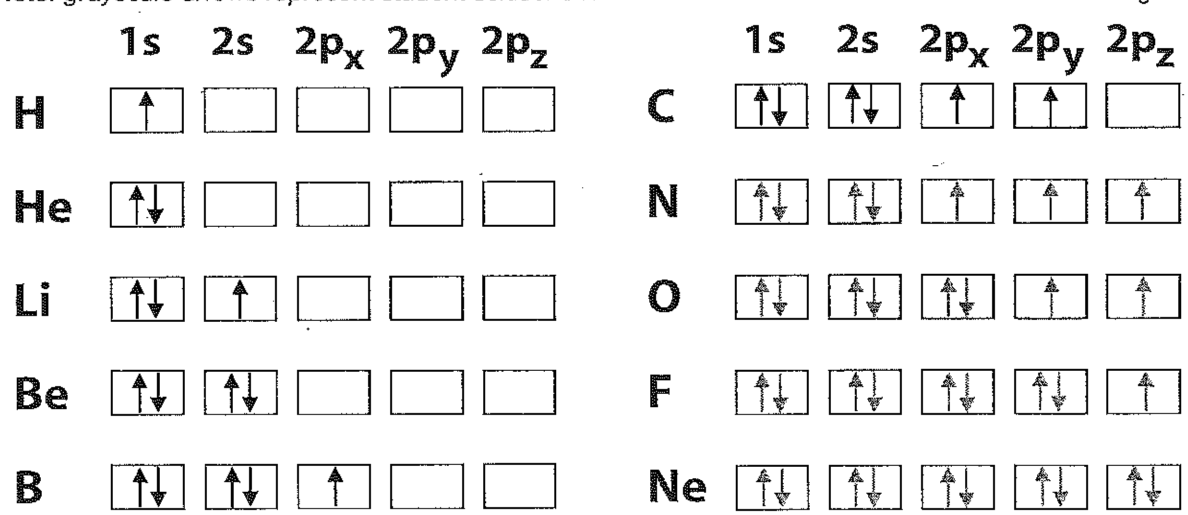
$$1s^2 2s^2 2p^2$$

This notation for the electron configuration means that 2 electrons are described by or are in the 1s orbital, 2 are in the 2s orbital, and 2 are in 2p orbitals. Electron configurations can also be represented by orbital box diagrams as shown below. In these diagrams an electron is represented by an upward or a downward pointing arrow. An upward pointing arrow indicates that the electron has positive spin angular momentum in one direction (referred to as *spin up*). A downward pointing arrow indicates that it has negative spin angular momentum in that direction (referred to as *spin down*). Dirac showed that the idea of spin angular momentum is a consequence of Einstein's theory of special relativity and does not mean that the electron is spinning like a top.

The following Key Questions will help you identify the principles or rules that account for the electron configurations by helping you examine the orbital box diagrams in Figure 1.

Note: grayscale arrows represent student solutions to Exercise 1

Figure1



Key Questions

1. Consider the orbital box diagrams in **Model 1**. Do electrons fill the lower or higher energy orbitals first?

   Electrons first fill the lower energy orbitals before they fill higher energy orbitals.

2. What is the maximum number of electrons that can go in each orbital?

Each orbital can accommodate two electrons.

3. If multiple orbitals with the same energy are available, e.g., in the case of 2p-orbitals, do the electrons all go in one orbital or do they go in different orbitals?

The electrons go in different orbitals until all orbitals have one electron. For example, there are three 2p orbitals. Although two electrons can be accommodated in each orbital, the Model shows that in carbon and nitrogen the electrons go into different orbitals before doubling up starting with oxygen.

4. According to the information in **Model 1**, how many different spin angular momentum states are there for each electron?

Each electron has two spin angular momentum states, corresponding to the upward pointing arrow (spin up) and the downward pointing arrow (spin down) in Figure 1.

KEY QUESTIONS

5. What are two ways shown in **Model 1** to write or specify the electron configuration of an atom?

*Electron configurations can be represented by a shorthand notation in which the principal number **n** is given, followed by a letter designating the angular momentum quantum number, and then the number of electrons shown by a superscript.*

Another way to represent electron configurations is through the use of an orbital diagram in which each orbital is drawn as a box which can accommodate two electrons. The electrons are shown as arrows, one up and one down, to indicate the electrons' spin angular momentum state.

6. What are the names of the three guidelines that determine the electron configuration of an atom?

Electron configurations are determined using the Pauli Exclusion Principle, the Aufbau Principle and Hund's Rule.

7. In the orbital box diagram for carbon shown in **Model 1**, why aren't both p-electrons in the p_x-orbital?

According to Hund's Rule, when multiple orbitals are available with the same energy, the orbitals first will be singly-filled by electrons with the same spin before electrons with different spins pair up within these orbitals. The electron configuration of lowest energy has the maximum number of unpaired electrons.

8. Why isn't the electron configuration of carbon $1s^3 2s^3$?

The s-orbital can accommodate a maximum of two electrons.

Exercises

Complete the orbital box diagrams in **Model 1** by applying the Aufbau Principle, the Pauli Exclusion Principle, and Hund's Rule.

Model 2: Electron-Electron and Electron-Nucleus Interactions in Atoms

Figure 2

Dominant Interparticle Forces in Helium

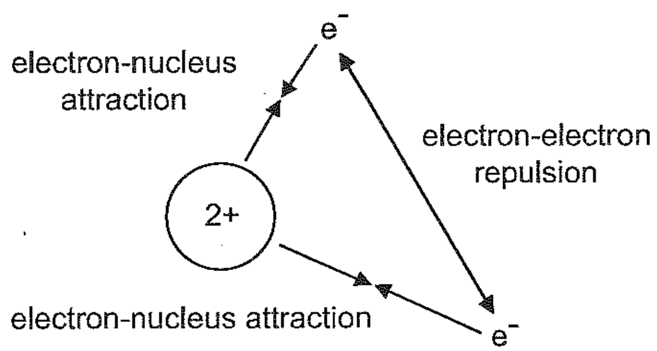
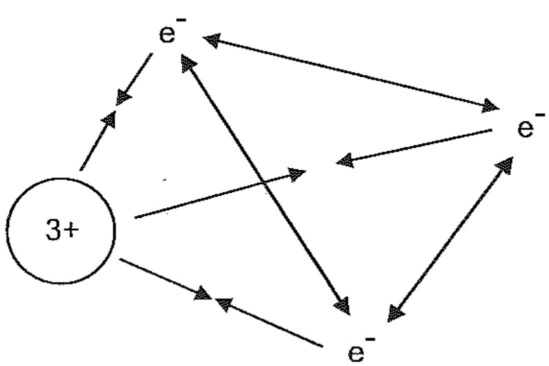


Figure 3

Dominant Interparticle Forces in Lithium



Note: *The diagrams in Figures 2 and 3 are not to scale. The nucleus is actually very much smaller relative to the placement of electrons (see Problem 2 in Activity 02-1).*

Information

The diagrams in **Model 2** illustrate how electron-electron repulsion can effectively reduce the attraction of an electron to the nucleus, and how this shielding effect depends on the electron configuration.

In helium, both of the electrons are in the same atomic orbital (1s) and therefore do not shield each other very well from the +2 charge of the nucleus. Consequently, the two electrons are strongly attracted to the nucleus.

In lithium, the outer electron is in a 2s orbital and is shielded very effectively from the +3 charge of the nucleus by the two electrons in the inner 1s orbital. As a result of this shielding and because it is farther from the nucleus, the outer electron experiences a smaller nuclear charge. Consequently, in lithium, the outer electron is not strongly attracted to the nucleus.

Key Questions

9. Is the electron-nucleus interaction attractive or repulsive? Explain.

   The electron-nucleus interaction is attractive because one is positively charged and the other is negatively charged. Opposite charges attract each other.

10. Is the electron-electron interaction attractive or repulsive? Explain.

    The electron-electron interaction is repulsive; both are negatively charged. Like charges repel each other.

11. Based on your interpretation of Figures 2 and 3, do you agree or disagree with the following statements? Explain your reasons for agreeing or disagreeing.

    a) Electrons in the same shell do not shield each other from the nuclear charge very effectively. So, for the case of helium, their attraction to the nucleus is characteristic of a nuclear charge less than, but close to, +2.

       This statement is correct. Electrons in the same shell do not shield each other from the nuclear charge very well.

    b) Electrons in inner shells are very good at shielding outer electrons from the nuclear charge. So, for the case of lithium, the electron-electron repulsion reduces the effective nuclear charge to a value much less than +3.

       This statement is correct. An outer shell electron is repelled by inner shell electrons. This repulsion significantly reduces the effective nuclear charge that the outer shell electron experiences.

Information

Ionization energy is defined as the energy required to ionize an atom and corresponds to the following reaction equation. (Ionization energy is a positive quantity.)

$$X \longrightarrow X^+ + e^-$$

By analogy, research scientists define *electron affinity* as the energy required to ionize an atomic anion. It corresponds to the following reaction equation. (Electron affinity is a positive quantity.)

$$Y^- \longrightarrow Y + e^-$$

In some general chemistry textbooks, the electron affinity is defined as the energy associated with the following electron attachment reaction.

$$Y + e^- \longrightarrow Y^-$$

Because this formula is just the reverse of the anion ionization reaction, this textbook convention produces an electron affinity with the same magnitude but a negative sign compared to the one used by research scientists.

Key Questions

12. Will an increase in the attraction to the nucleus tend to increase or decrease each of the following? Explain.

    a) The size of an atom

       Decrease: An increased attraction to the nucleus draws electrons in and results in a small atomic radius.

    b) The ionization energy

       Increase: An increased attraction to the nucleus requires a greater ionization energy.

    c) The electron affinity

       Increase: Stronger nuclear attraction also increases the energy needed to remove an electron from the anion.

13. Will an increase in the repulsion of an electron by other electrons tend to increase or decrease each of the following? Explain.

    a) The size of an atom

       Increase: Increased repulsive forces push electrons farther away from each other and away from the nucleus increasing the atomic radius.

    b) The ionization energy

       Decrease: Since electrons are pushed away from the nucleus, the attraction to the nucleus becomes weaker; therefore these electrons are less tightly held by the nucleus and the ionization energy decreases.

    c) The electron affinity

       Decrease: Increased repulsive forces mean that the additional electron in the anion is less tightly held by the nucleus and the atom has a smaller electron affinity.

Exercises

2. In going from hydrogen to helium, there is a change in the atomic radius (from 37 to 32 pm) and a change in ionization energy (from 1311 kJ/mole to 2377 kJ/mole). Identify what these changes suggest about the relative magnitudes of the changes in the *electron–nucleus attraction* and the *electron–electron repulsion.*

   In going from H to He, an electron was added, and the nuclear charge increased by 1 unit. The added electron produces electron-electron repulsion, and the increase in nuclear charge increases the electron-nucleus attraction. Since He is smaller than H and has a higher ionization potential, it appears that the increased electron-nucleus attraction has the larger effect.

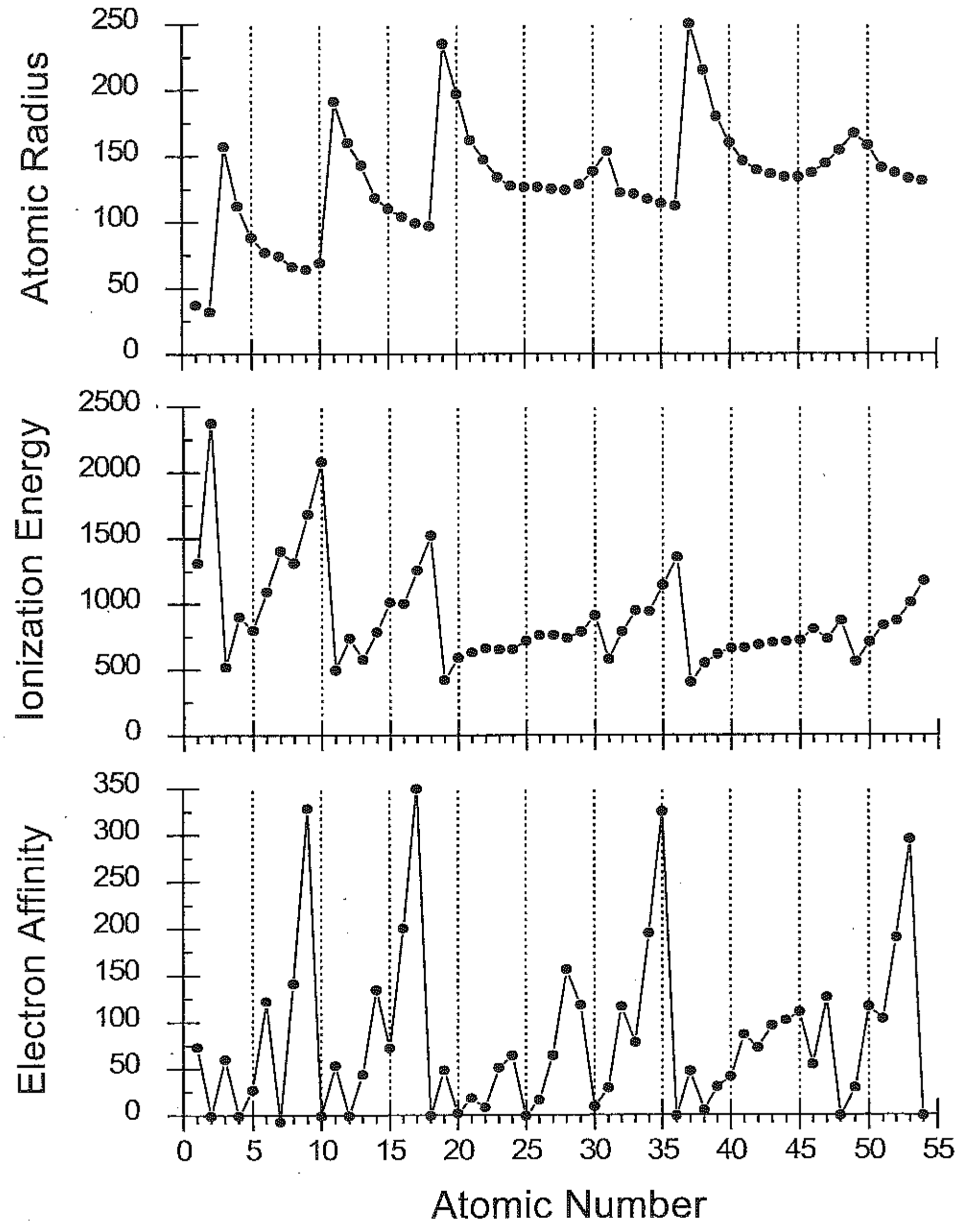
3. Using the ideas illustrated in **Model 2** and developed by the preceding Key Questions and Exercise 2, explain why you would you expect lithium to be larger and have a smaller ionization energy than helium.

   The 2s electron in Li is in an outer shell and is farther away from the nucleus than are the 1s electrons in He. The 2s electron in Li is also repelled by the two 1s electrons that lie between it and the nucleus. Both of these effects (farther away and repelled) are expected to make Li larger and have a smaller ionization energy than He.

MODEL 3: VARIATION OF ATOMIC PROPERTIES WITH ATOMIC NUMBER

The unit for atomic radii is pm; the unit for ionization energies and electron affinities is kJ/mole.

Figure 4



KEY QUESTIONS

14. The Periodic Table is organized with the atomic number of the elements increasing from the beginning to the end. Similarly, the x-axis for all graphs in **Model 3** is the atomic number of the element. In going from one element to the next across the x-axis, what happens to the number of protons and the number of electrons?

The numbers of protons and electrons both increase by 1 from one element to the next.

15. Do additional protons tend to increase or decrease the electron-nucleus attraction? Explain.

    Additional protons increase the electron-nucleus attraction since the attractive force is proportional to the nuclear charge.

16. Do additional electrons tend to increase or decrease the electron-electron repulsion? Explain.

    Additional electrons increase the amount of electron-electron repulsion since each electron repels all of the other electrons.

17. Using the information from the graphs in **Model 3**, describe what happens to the atomic radius and ionization energy as you go across a row in the Periodic Table, e.g., from Li to Ne and Na to Ar?

    The atomic radius of an atom decreases as one proceeds across a period from left to right, and ionization energy generally increases.

18. Why do the trends that you identified in Key Question 17 occur? In your explanation use the increase in nuclear charge and the effectiveness of electron shielding of the nuclear charge by electrons in the same orbital as illustrated in **Model 2**.

    The atomic radius of an atom decreases and the ionization energy generally increases, as one proceeds across a period from left to right because protons are added to the nucleus. Electrons are added as well, but the electrons are added to the same shell and are only moderately effective at repelling the other electrons or shielding them from the nuclear charge. Therefore increasing the nuclear charge has a larger effect than increasing the number of electrons, and the radii decrease and ionization energies increase.

19. Using the information from the graphs in **Model 3**, describe what happens to the atomic radius and ionization energy when going down a group in the Periodic Table, such as from Ne to Xe or Li to Rb.

    As one proceeds down a group in the periodic table, the atomic radius increases and the ionization energy decreases.

20. Why do the trends that you identified in Key Question 19 occur? In your explanation, use the increase in nuclear charge, the effect of electron shielding of the nuclear charge by electrons in inner shells, and the size of the outer shell.

    In going down a group in the Periodic Table, the radius of the outermost orbital increases and the attraction of an electron for the nucleus decreases because of this larger distance. Also the inner shell electrons are very good at repelling the outermost electrons and shielding them from the increased nuclear charge. Consequently the attraction for the nucleus is greatly reduced, and the atomic radius increases and the ionization energy decreases.

21. How can you use the Periodic Table and electron configurations to predict relative atomic radii and ionization energies for two atoms?

*Each group in the Periodic Table has the same electron configuration but with different values for the principal quantum number **n**. Within a group, an atom with the larger value of **n** will be larger and have a lower ionization energy for reasons discussed in response to Key Question 20.*

If the principal quantum number is the same for two atoms (same row in the Periodic Table), then increasing the number of protons increases the attraction to the nucleus to a greater extent than the increase in the repulsion or shielding by the additional electrons in the same shell. This difference between the increase in attraction and repulsion results in a decreasing radius and an increasing ionization energy moving from left to right across a row in the Periodic Table

EXERCISES

4. Identify the larger of each pair, and explain why that one is larger.

calcium or potassium

Ca $1s^22s^22p^63s^23p^64s^2$

K $1s^22s^22p^63s^23p^64s^1$

Potassium is larger than calcium. Both have electrons in orbitals in the fourth shell. Potassium has 19 protons and calcium has 20 protons; thus calcium has a greater nuclear charge. Calcium's increased nuclear charge allows it to draw its electrons closer to the nucleus, resulting in a smaller size because the electron-electron repulsion by electrons in the same shell is not able to cancel out or shield the increased nuclear charge.

nitrogen or oxygen

N $1s^22s^22p^3$

O $1s^22s^22p^4$

Nitrogen is larger than oxygen. Both have electrons in orbitals in the second shell. Nitrogen has 7 protons and oxygen has 8 protons; thus oxygen has a greater nuclear charge. Oxygen's increased nuclear charge allows it to draw its electrons closer to the nucleus, resulting in a smaller size because the electron-electron repulsion by electrons in the same shell is not able to cancel out or shield the increased nuclear charge.

sodium or potassium

Na $1s^22s^22p^63s^1$

K $1s^22s^22p^63s^23p^64s^1$

Potassium is larger than sodium because the 4s electron is farther from the nucleus than the 3s electron in sodium. Even though potassium has a larger nuclear charge than sodium, this charge is balanced by the larger number of electrons so the effective nuclear charge is essentially the same for both potassium and sodium.

5. Identify which of the elements in each pair has the higher ionization energy, explaining why for each.

Ba or Cs

Ba $1s^22s^22p^63s^23p^64s^23d^{10}4p^65s^24d^{10}5p^66s^2$

Cs $1s^22s^22p^63s^23p^64s^23d^{10}4p^65s^24d^{10}5p^66s^1$

Barium has the higher ionization energy. Both barium and cesium have electrons in orbitals in the sixth shell. Cesium has 55 protons and barium has 56 protons; thus barium has a greater nuclear charge. This difference causes the outermost electrons in barium to experience a greater electron-nuclear attraction than the electrons in cesium because the electron-electron repulsion by electrons in the same shell is not able to cancel out or shield the increased nuclear charge.

Br or Kr

Br $1s^22s^22p^63s^23p^64s^23d^{10}4p^5$

Kr $1s^22s^22p^63s^23p^64s^23d^{10}4p^6$

Krypton has the higher ionization energy. Both bromine and krypton have electrons in orbitals in the fourth shell. Bromine has 35 protons and krypton has 36 protons; thus krypton has a greater nuclear charge. This larger charge causes the outermost electrons in krypton to experience a larger electron-nuclear attraction than the electrons in bromine because the electron-electron repulsion by electrons in the same shell is not able to cancel out or shield the increased nuclear charge.

Si or C

Si $1s^22s^22p^63s^23p^2$

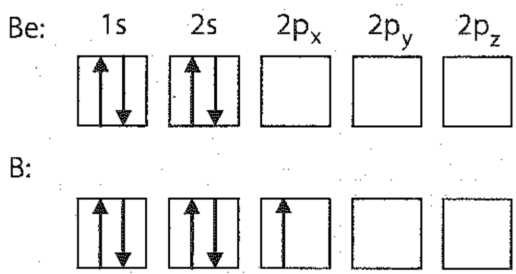
C $1s^22s^22p^2$

Carbon has the greater ionization energy. The electrons in the $n = 3$ *shell of silicon are farther from the nucleus than are the electrons in the* $n = 2$ *shell of carbon and thus less strongly attracted to the nucleus because of this larger distance. The larger number of protons in the silicon nucleus is cancelled by the shielding effect of the inner shell electrons. Thus carbon has the larger effective nuclear charge and its ionization energy is greater.*

PROBLEMS

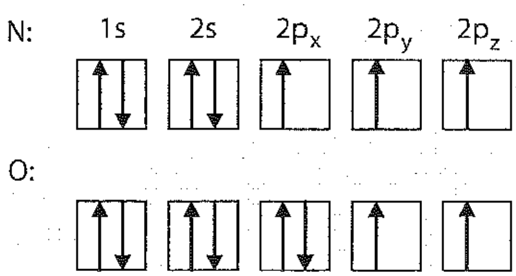
1. In the Periodic Table, ionization energies tend to increase across a period or row. For the ionization energies in the second period (Li to Ne), identify where the exceptions to this general trend occur. To help you explain these exceptions, use orbital box diagrams like those in **Model 1** and your knowledge of the differences in electron configurations between neighboring atoms.

   There is an exception to the trend for ionization energies between Be and B. The orbital diagrams are shown below:



   Removing a single 2p electron from B requires less energy than removing an electron from the filled 2s sub-shell in Be. The 2p electron in boron is shielded by both the 1s and the 2s electrons, decreasing electron-nuclear attractions and resulting in an electron that is more easily removed. Removal of one of the 2s electrons from Be requires more energy because there is less shielding and a greater effective nuclear charge.

   Another exception can be found between nitrogen and oxygen. The orbital diagrams are shown below:



   It requires less energy to remove the fourth electron from the 2p orbital in oxygen than to remove the third electron from the 2p orbital of nitrogen. Placing a second electron in the same orbital results in a much greater electron-electron repulsion (in oxygen) than placing electrons in separate orbitals (in nitrogen). The increased repulsion reduces the energy required to ionize oxygen even though there is an increase in nuclear charge.

2. Using the insight you gained from Problem 1, explain:

   a) Why the first ionization energy of sulfur is less than the first ionization energy of phosphorus.

   S $1s^2 2s^2 2p^6 3s^2 3p^4$

   P $1s^2 2s^2 2p^6 3s^2 3p^3$

   It requires less energy to remove the fourth electron from the 3p orbital in sulfur than to remove the third electron from the 3p orbital of phosphorus. The effect is exactly the same as described for N and O (from the second Period) in Problem 1 (above).

   b) Why the first ionization energy of aluminum is less than the first ionization energy of magnesium.

   Al $1s^2 2s^2 2p^6 3s^2 3p^1$

   Mg $1s^2 2s^2 2p^6 3s^2$

   Removing a single 3p electron from Al requires less energy than removing an electron from the filled 3s sub-shell in Mg. The effect is exactly the same as described for Be and B (from the second period) in Problem 1 (above).

3. Variations in electron affinities can be understood in the same way that variations in ionization energies are understood; except that, in the analysis of the effects of electron shielding and nuclear charge, one uses the electron configuration and the orbital box diagram for the anion rather than for the atom. Using this idea, identify the atom in each pair that has the greater electron affinity and explain why.

H or He

H^- $1s^2$

He^- $1s^2 2s^1$

Hydrogen has a greater electron affinity than helium. In hydrogen the additional electron to produce the anion goes into the 1 s orbital and is not shielded very well from the nuclear charge of +1 by the other electron in the 1s orbital.

In helium the additional electron to produce the anion goes into the 2s orbital and is shielded very well by the two 1s electrons. Complete shielding would mean that the effective nuclear charge for the 2 s electron is 0, so the additional electron would not be bound at all.

He or Li

He^- $1s^2 2s^1$

Li^- $1s^2 2s^2$

Lithium has a greater electron affinity than helium. In helium the electron goes into the 2s orbital and is shielded very well from the +2 nuclear charge by the two 1s electrons. In lithium the electron joins another electron in the 2s orbital and the shielding of the +3 charge is effective by the two electrons in the 1s orbital but not so effective by the other electron in the 2s orbital because they are in the same shell.

B or C

B^- $1s^2 2s^2 2p^2$

C^- $1s^2 2s^2 2p^3$

Carbon has a greater electron affinity than boron. Carbon has a nuclear charge of +6 and boron has a nuclear charge of +5. In both atoms, there are 4 inner electrons that strongly shield the extra electron from the nucleus, so the effective nuclear charge is expected to be larger for carbon than for boron.

Cl or Ar

Cl^- $1s^2 2s^2 2p^6 3s^2 3p^6$

Ar^- $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

Cl has a greater electron affinity than Ar. The additional electron in argon is in the a n = 4 outer shell and is strongly repelled or shielded by all the other 18 electrons in the n = 1, 2, and 3 shells. In the case of chlorine the strong repulsion and shielding only involves the 10 electrons in the n = 1 and 2 shells.