

Chapter 2 – Quantum Theory

Introduction

Quantum theory explains our world at the atomic and molecular levels. A few brilliant scientists, who were trying to explain the results of experiments that defied the physics of the day, launched a theory that would change our view of not only the atom and the molecule, but of the universe as well. In this chapter, some of the key experiments leading to quantum theory are described, and then the theory is applied to the electrons in an atom.

2.1 The Nature of Light

Introduction

Although we do not see atoms and molecules, much of our understanding of them is based on the way they interact with light. This lesson deals with the nature of light.

Objectives

- Describe the relationship between the speed, wavelength, and frequency of a light wave.
- Determine the relative wavelengths and frequencies of two light waves given the region of the electromagnetic spectrum in which they lie.

2.1-1. Wavelength

Light is electromagnetic radiation; that is, it is an oscillating electric and magnetic field that travels through space at a constant speed, $c = 2.998 \times 10^8$ m/s, the speed of light. The electric and magnetic fields are perpendicular to one another, but only the electric field is shown in the figures in this section.

A light wave is characterized by its amplitude, which is the distance between the valley and the peak of the wave, and its **wavelength**, λ , which is the distance between two adjacent maxima or minima in the electric (or magnetic) field. The amplitude indicates the brightness of the light, and the wavelength tells us what kind of light it is.

Visible light, the light visible to the human eye, is only a small fraction of all electromagnetic radiation, and the different colors that we see differ because they have different wavelengths. Red light has the longest wavelength in the visible region and violet light has the shortest.

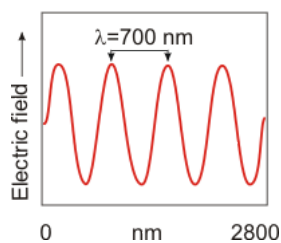


Figure 2.1a: A 2800-nm Segment of Red Light Red light has the longest wavelength of visible light. The red wave shown here has a wavelength of 700 nm. The 2800-nm segment contains four wavelengths of red light.

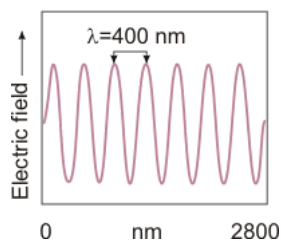


Figure 2.1b: A 2800-nm Segment of Violet Light Violet light has the shortest wavelength of visible light. The violet wave shown here has a wavelength of 400 nm. The 2800-nm segment contains seven wavelengths of violet light.

Note that both figures show a segment of wave that is 2800 nm in length. However, the two segments contain a different number of wavelengths. Thus, the waves are more *frequent* in the violet wave. Indeed, this property, called the frequency of the light, is another very important characteristic of the light wave that is taken up next.

2.1-2. Frequency

The product of the wavelength and frequency of a light wave equals the speed of light.

Electromagnetic radiation can also be characterized by its **frequency**, ν . The frequency of a light wave is the number of oscillations of the electromagnetic field per second (i.e., the number of waves that pass a point per second). How many waves that pass the point depends upon how fast the wave is moving and how close the waves are to one another. All light waves travel at the same speed (c) and the distance between the waves is the wavelength (λ). Thus, a shorter wavelength means closely packed waves, which means that more waves will pass per second (i.e., the greater the frequency of the light). The speed (c), frequency (ν), and the wavelength (λ) of light are related by the following expression.

$$c = \nu\lambda \quad (2.1)$$

As shown in the above expression, the frequency of a light wave increases as its wavelength decreases. This is demonstrated below where the frequencies of red and violet light are compared.

EXAMPLE:

As an example, consider the frequencies of violet ($\lambda = 400 \text{ nm} = 4 \times 10^{-7} \text{ m}$) and red light ($\lambda = 700 \text{ nm} = 7.00 \times 10^{-7} \text{ m}$), which would be calculated as follows.

$$\nu_{\text{violet}} = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m} \cdot \text{s}^{-1}}{4.00 \times 10^{-7} \text{ m}} = 7.50 \times 10^{14} \text{ s}^{-1}$$

$$\nu_{\text{red}} = \frac{c}{\lambda} = \frac{3.00 \times 10^8 \text{ m} \cdot \text{s}^{-1}}{7.00 \times 10^{-7} \text{ m}} = 4.29 \times 10^{14} \text{ s}^{-1}$$

2.1-3. Electromagnetic Spectrum

An electromagnetic **spectrum** is a display of the component colors of a light beam, separated by their wavelengths. Raindrops can sometimes separate the component colors of white light by their wavelengths to produce a rainbow, which is a display of the spectrum of white light. Because the colors all merge into one another continuously, the resulting spectrum is called a **continuous spectrum**. A continuous spectrum can also be obtained by dispersing white light through a prism or from a grating. It should be noted that the visible region of the electromagnetic spectrum (that portion the eye can perceive) is but a small part of the entire spectrum. Further information about the EM spectrum can be found at http://imagine.gsfc.nasa.gov/docs/science/know_l1/emspectrum.html¹.

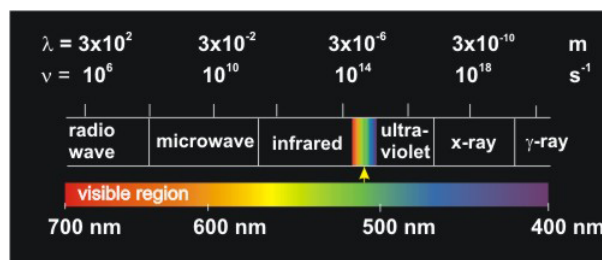


Figure 2.2: The Electromagnetic (EM) Spectrum The visible region (400 – 700 nm), which is a very small portion of the spectrum, is expanded.

¹http://imagine.gsfc.nasa.gov/docs/science/know_l1/emspectrum.html

2.2 Quantization

Introduction

In this lesson, we introduce the concept of quantization, i.e., that energy comes in small packets called quanta.

Objectives

- Define the terms *quantized* and *photon*.
- Calculate the energy of a photon from its frequency.
- Explain what is meant by ‘wave-particle duality.’
- Define continuous spectrum and describe the spectrum of white light.
- Use the Rydberg equation to determine the frequency of a spectral line from the quantum numbers of the levels involved.

Blackbody Radiation

2.2-1. Blackbody Radiation Experiment

All objects emit electromagnetic waves, and as their temperature increases, so too do the total intensity and the average frequency of the radiation. At sufficiently high temperatures, a significant portion of the radiation is in the visible region of the spectrum. For example, a burner in an electric oven emits invisible but warm infrared radiation on a low setting, but it becomes ‘red hot’ on a high setting as it emits both infrared and visible radiation. Similarly, the tungsten filament of a light bulb becomes ‘white hot’ because all of the colors in the visible region are being emitted. This emission of electromagnetic waves from a warm body is called blackbody radiation.

A video or simulation is available online.

2.2-2. Blackbody Radiation Explanation

A photon is a bundle of light energy, which is proportional to the frequency of the light.

The model used by physicists in the late 1800s assumed that the energy of a wave depended only upon its amplitude (intensity), so each light wave that was emitted by a blackbody radiator was thought to contain the same amount of energy. Since an infinite number of waves were allowed and each wave had the same energy, the model predicted that there should be an infinite amount of energy given off!

Max Planck discovered that the infinite energy dilemma was removed if the energy of a wave is quantized. That is, the total energy of a wave could not be varied continuously because it is composed of many tiny bundles of energy called quanta. Quanta of light are called photons. Thus, a light wave is comprised of photons much like a wave of water is comprised of water molecules except that photons do not have mass. The energy of one **quantum** of light (photon) depends only upon its frequency. That is,

$$E = h\nu \tag{2.2}$$

where $h = 6.626 \times 10^{-34}$ J-s is called **Planck’s constant**. The amount of energy in a wave that contains n quanta (photons) is then the following.

$$E = nh\nu$$

Planck’s model for the quantization of wave energy correctly accounted for blackbody radiation, but the only reason he could offer for proposing this remarkable behavior was that it worked.

2.2-3. Photon Energy Exercise

EXERCISE 2.1:

What are the energies of the following in Joules? Express small numbers with the e format, e.g., 1.23e-12.

a photon red with a frequency of $4.60 \times 10^{14} \text{ s}^{-1}$ _____ J

a mole of photons with frequency of $4.60 \times 10^{14} \text{ s}^{-1}$ _____ J

The Photoelectric Effect

2.2-4. The Photoelectric Effect Experiment

Another observation of the late 1800s that could not be understood with the classical picture of light was that certain metals, when irradiated with light, ejected electrons. The kinetic energy of the electrons depended only upon the metal and the frequency of light. Increasing the intensity of the light increases the number of electrons that are ejected, but not their kinetic energy. For these metals, there is a minimum frequency below which no electrons are ejected, no matter how intense the light. This minimum frequency is called the threshold frequency of the metal, ν_0 . As shown in Figure 2.3, a plot of the ejected electron's kinetic energy versus the frequency of the light striking the metal is a straight line.

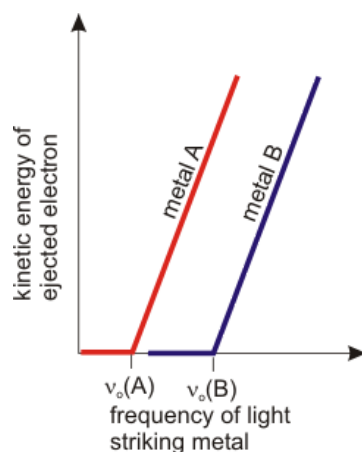


Figure 2.3: Photoelectric Effect No electrons are ejected when a metal is irradiated with light at frequencies below the threshold frequency (ν_0). At frequencies above the threshold frequency of the metal, electrons are ejected with a kinetic energy that increases linearly with the frequency of the light.

2.2-5. The Photoelectric Effect Explanation

In order to explain the photoelectric effect, Albert Einstein used Planck's hypothesis that light was composed of energy quanta. He proposed that light consisted of particles of energy, which we now call **photons**, each with an energy $h\nu$. He reasoned that, if the electrons are bound to a metal by an energy, W , then the threshold frequency for electron ejection from a metal (ν_0) is that frequency for which $h\nu_0 = W$. When the frequency (energy) of the photon is less than the threshold frequency of the metal, electrons cannot be removed because the energy that binds them to the metal is greater than the energy of the photon. However, when the energy of each photon exceeds the energy that binds the electron to the metal ($h\nu > W$), the energy of the photon is transferred to the electron. A portion of the photon's energy, W , is used to overcome the potential energy binding the electron to the metal and the excess energy is converted into the kinetic energy of the ejected electron (KE).

$$KE = h\nu - W = h\nu - h\nu_0$$

According to Einstein, the intensity of a light wave reflects the number of photons that it contains. A beam that contains n photons has a total energy of $n h\nu$, but when light interacts with matter, it does so one photon at a time. Thus, it is the energy of each photon that dictates the energy of a molecular process that is initiated by the light,

while the number of events that occur per unit time, i.e., the rate of the process is dictated by the intensity of the light.

Planck and Einstein had shown that light consisted of particles of energy called photons, but classical experiments showed that light is also a wave. This property of behaving as both a particle and a wave is called ***wave-particle duality***.

Atomic Spectra

2.2-6. Continuous Spectrum

All wavelengths of visible light are present in white light, so when white light is dispersed as shown in Figure 2.4, the colors merge into one another continuously to produce a continuous spectrum.

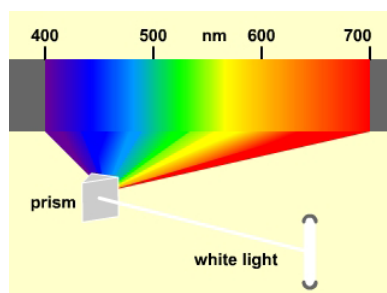


Figure 2.4

2.2-7. Gas Discharge Tubes

A gas discharge tube is an evacuated tube that has been filled with a gas at low pressure. When high-energy electrons are passed through a discharge tube (a high voltage is placed across it), the tube glows with a color that is characteristic of the gas. As shown in Figure 2.5, a neon light has a characteristic red color, while a gas discharge tube filled with hydrogen glows with purple-blue color.

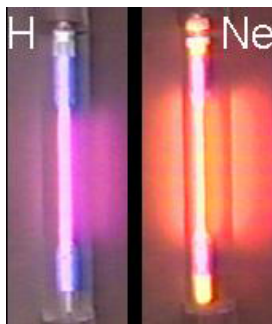


Figure 2.5

The color of the glow from a hydrogen discharge tube is not white, so not all wavelengths of visible light are present. This means that when this light is dispersed, many of the wavelengths present in the continuous spectrum of white light are missing. We examine the hydrogen spectrum in the following section.

2.2-8. Line Spectra

Atomic spectra are line spectra.

The colors observed in the spectrum of a gas discharge tube do not merge into one another. Instead the spectra consist of series of lines. Since the colors are observed as lines, the spectra are called ***line spectra***. The purple-blue color of the hydrogen discharge is due to the presence of light of only four different wavelengths of visible light as shown in Figure 2.6.

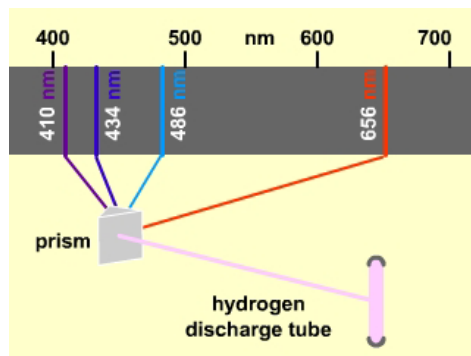


Figure 2.6: Line Spectrum of Hydrogen When the glow from a hydrogen discharge tube is focused down to the image of a slit and passed through a prism, it is broken down into four component wavelengths: 410 nm (violet), 434 nm (blue), 486 nm (green), and 656 nm (red). The four colors are observed as lines in the visible spectrum of hydrogen. However, there are over forty such lines observed throughout the ultraviolet, the visible, and the infrared.

Each element has a characteristic spectrum that can be used to identify the element. Visit a site at the University of Oregon² to view line spectra of the elements. The default is the absorption spectrum, so be sure to select 'emission'. Then click on an element. You can even determine the wavelengths of the lines by clicking in the spectrum. The number that appears is in **Angstroms**, so divide it by 10 to get nanometers.

- 1 Look at Ne and compare the spectrum to the color of a neon light.
- 2 Verify that Lithium has a strong line at 610 nm.
- 3 Examine the spectra of the alkali metals. What general statement can be made about how the spectra of the atoms change as you proceed down a group?

2.2-9. Calculating the Line Spectrum of Hydrogen

Scientists did not understand the origin of line spectra, but Johannes Rydberg found a relatively simple mathematical expression, called the **Rydberg equation** and shown as Equation 2.3a below, that allowed him to calculate the frequency of every line in the hydrogen spectrum (over 40 lines). Multiplication of frequency in the Rydberg equation by Planck's constant yields the energy of the emitted photon in joules ($E = h\nu$) as shown in Equation 2.3b.

$$\nu = R_H \left(\frac{1}{n_{lo}^2} - \frac{1}{n_{hi}^2} \right) = 3.290 \times 10^{15} \left(\frac{1}{n_{lo}^2} - \frac{1}{n_{hi}^2} \right) \text{ s}^{-1} \quad (2.3a)$$

$$E_{\text{photon}} = h\nu = hR_H \left(\frac{1}{n_{lo}^2} - \frac{1}{n_{hi}^2} \right) = 2.180 \times 10^{-18} \left(\frac{1}{n_{lo}^2} - \frac{1}{n_{hi}^2} \right) \text{ J} \quad (2.3b)$$

- ν is the frequency of the emitted photon in s^{-1} .
- E_{photon} is the energy of the emitted photon with frequency ν .
- $n_{lo} < n_{hi}$ are positive integers.
- $R_H = 3.290 \times 10^{15} \text{ s}^{-1}$ is the Rydberg constant for hydrogen.

2.2-10. Rydberg Exercise

EXERCISE 2.2:

Use Equation 2.3a to determine the frequencies and wavelengths of the following spectral lines. Indicate whether each line falls in the infrared, visible, or ultraviolet region of the electromagnetic spectrum.

$$n_{lo} = 2, n_{hi} = 4 \quad \nu = \text{_____} \text{ s}^{-1}$$

$$n_{lo} = 2, n_{hi} = 4 \quad \lambda = \text{_____} \text{ nm}$$

²<http://jersey.uoregon.edu/vlab/elements/Elements.html>

$n_{\text{lo}} = 2, n_{\text{hi}} = 4$ region:

infrared

visible

ultraviolet

$n_{\text{lo}} = 1, n_{\text{hi}} = 2 \quad \nu = \text{_____} \text{ s}^{-1}$

$n_{\text{lo}} = 1, n_{\text{hi}} = 2 \quad \lambda = \text{_____} \text{ nm}$

$n_{\text{lo}} = 1, n_{\text{hi}} = 2$ region:

infrared

visible

ultraviolet

$n_{\text{lo}} = 4, n_{\text{hi}} = 7 \quad \nu = \text{_____} \text{ s}^{-1}$

$n_{\text{lo}} = 4, n_{\text{hi}} = 7 \quad \lambda = \text{_____} \text{ nm}$

$n_{\text{lo}} = 4, n_{\text{hi}} = 7$ region:

infrared

visible

ultraviolet

2.3 Bohr Model

Introduction

In the Rutherford model, electrons moved in circular orbits, but particles tend to move in straight lines not circles, so circular orbits require a force, called the centripetal force, to pull the orbiting particle toward the center. Earth is kept in its orbit by the gravitational attraction of the sun, and the electron is kept in its orbit by the Coulombic attraction of the nucleus. However, there was one major flaw with these orbiting electrons: the orbit would be unstable because a charged particle moving in this way would radiate energy, which would cause it to spiral into the nucleus, but clearly that was not the case in the hydrogen atom!

Prerequisites

- 1.8 Electromagnetism and Coulomb's Law (Relate the energy of interaction between two charged particles to the distance separating them.)

Objectives

- Relate energy of an electron to its n quantum number and the nuclear charge.
- Draw an energy level diagram for the hydrogen atom that shows the relative separations between the energy levels.

2.3-1. Bohr Radius

Note that the discussions of this section all ignore interactions between electrons, so they pertain only to systems that involve a **single** electron interacting with a nucleus with Z protons. Thus, the discussions are relevant to a H atom ($Z = 1$), but they do not apply to other atoms because all other atoms contain more than one electron. However, they do apply to the one-electron ions of other atoms such as He^{1+} , Li^{2+} , Be^{3+} , etc.

Niels Bohr³, a Danish physicist, postulated the reason for the stability of the atom: the electron remains in its orbit because its angular momentum is quantized. He proposed that the angular momentum was proportional to an integer, called the principal quantum number, n ($n = 1, 2, 3, 4, \dots$). By forbidding $n = 0$, he assured that the electron always had some angular momentum, which stabilized the orbit and kept the electron moving in its circular path! He used Coulomb's Law to evaluate the electron-nuclear attraction (F_e in Figure 2.7) and the quantized angular momentum to determine the centripetal force (F_c in Figure 2.7). He then equated the two forces to determine the stable radii of rotation to be the following.

³http://www.groups.dcs.st-and.ac.uk/~history/Mathematicians/Bohr_Niels.html

$$r_n = (5.292 \times 10^{-11}) \left(\frac{n^2}{z} \right) \text{ m} = (52.92) \left(\frac{n^2}{z} \right) \text{ pm} \quad (2.4)$$

The n^2 dependence expressed of the radius that appears in the equation is shown in Figure 2.7. The constant (52.92 pm) was calculated from known physical constants, such as Planck's constant, and the mass and charge of the electron and the proton. Z is the atomic number (number of positive charges in the nucleus). For a hydrogen atom, $n = 1$ and $Z = 1$, so the distance between the electron and the proton was determined to be $r_1 = 52.92$ pm, which is called the Bohr radius.

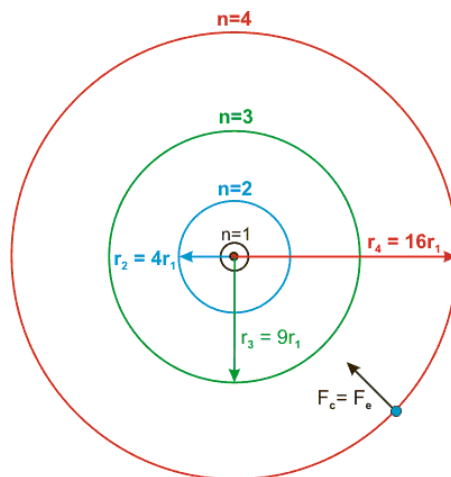


Figure 2.7: Relative Radii of First Four Bohr Orbits $r_1 = 52.92$ pm, and $r_n = n^2 r_1$

2.3-2. Electron Energy

The energy of an electron in an atom is quantized, so electrons are said to occupy energy levels.

The total energy of the electron (E) is the sum of its kinetic energy (KE) and its potential energy (U); i.e., $E = KE + U$. The potential energy of the electron in a one-electron system arises from its Coulombic energy of interaction with the nucleus, and its kinetic energy from its circular motion about the nucleus. However, the fact that the centripetal force resulted from the Coulombic force required that the kinetic energy be one-half of the Coulombic energy but opposite in sign (i.e., $KE = -1/2U$). The total energy is then $E = KE + U = -1/2U + U = 1/2U$. The Coulombic energy of interaction between the nucleus and the electron is given by Coulomb's Law (Equation 1.2), so the total energy of an electron in the n^{th} orbit is the following.

$$E_n = \frac{1}{2}U_n = \frac{1}{2} \left(\frac{kq_e q_N}{\epsilon r_n} \right)$$

The basic unit of charge is $q = 1.602 \times 10^{-18}$ C, so the charge on an electron is $q_e = -q$ and the charge on a nucleus with Z protons is $q_N = +Zq$. The value of ϵ in a vacuum is one, and r is the radius of the n^{th} orbit as given in Equation 2.4. Substitution of these known quantities into the preceding energy expression yields the total energy of an electron in the n^{th} orbit in terms of the n quantum number.

$$E_n = (-2.180 \times 10^{-18}) \left(\frac{Z^2}{n^2} \right) \text{ J} = (-hR_H) \left(\frac{Z^2}{n^2} \right) \quad (2.5)$$

The constant determined by Bohr, 2.180×10^{-18} J, was the same as the experimental value determined by Rydberg for hR_H in Equation 2.3b (i.e., $2.180 \times 10^{-18} = hR_H$). This agreement with experiment was strong support for the Bohr model.

The energy associated with each value of n in Equation 2.5 is called an **energy level**. In the case of a hydrogen atom, $Z = 1$, so the energy of the $n = 1$ level is -2.180×10^{-18} J, and that of the $n = 2$ level is $-2.180 \times 10^{-18} (1^2/2^2) = -5.450 \times 10^{-19}$ J. The energies are negative because the energy of an electron in an atom is less than that of a free electron.

2.3-3. Bohr Model Exercise

EXERCISE 2.3:

Use the Bohr model to determine the orbital radius and energy of an electron in the $n = 1$ level of a Li^{2+} ion. We use the $+2$ ion because the Bohr model only applies to species with one electron.

$Z =$ _____

$n =$ _____

$r_n =$ _____ pm

$E_n =$ _____ J

2.3-4. Energy Level Diagram

Atomic spectra can be understood in terms of the electron moving from one energy level into another, which is referred to as an **electronic transition**. If n_{hi} is the higher quantum number and n_{lo} is the lower quantum number, then the energy difference between the two energy levels is $\Delta E = E_{n_{\text{hi}}} - E_{n_{\text{lo}}}$, which can be determined with Equation 2.5 to be the following.

$$\Delta E_{\text{atom}} = E_{n_{\text{hi}}} - E_{n_{\text{lo}}} = -hR_{\text{H}}Z^2 \left(\frac{1}{n_{\text{hi}}^2} - \frac{1}{n_{\text{lo}}^2} \right) = hR_{\text{H}}Z^2 \left(\frac{1}{n_{\text{lo}}^2} - \frac{1}{n_{\text{hi}}^2} \right) \quad (2.6)$$

ΔE_{atom} in Equation 2.6 is identical to E_{photon} in the empirical Equation 2.3b. Thus, an electron's energy can change by ΔE_{atom} by either absorbing or emitting a photon with an energy of E_{photon} .

- **Absorption:** a photon is absorbed if n_{lo} is the initial level. The absorption of energy increases the energy of the electron to the level of n_{hi} .
- **Emission:** a photon is emitted if n_{hi} is the initial level. The emission of energy decreases the energy of the electron to the level of n_{lo} .

The electronic transitions resulting in some of the 40 lines in the emission spectrum of a hydrogen atom are represented with the vertical arrows in Figure 2.8. The lowest energy line in the visible series occurs for $n_{\text{lo}} = 2$ and $n_{\text{hi}} = 3$, which is designated as the $n = 3 \rightarrow 2$ transition ($3 \rightarrow 2$). The violet line in the H atom spectrum is the highest energy line in the visible region; it results from the $6 \rightarrow 2$ transition. Note that the lines would correspond to absorptions if the arrows were pointed in the opposite direction. For example, the $2 \rightarrow 3$ transition is an absorption because the initial level is n_{lo} . Note the following for hydrogen atom spectrum:

- $n_{\text{lo}} = 1$ for all lines in the ultraviolet region.
- $n_{\text{lo}} = 2$ for all lines in the visible region.

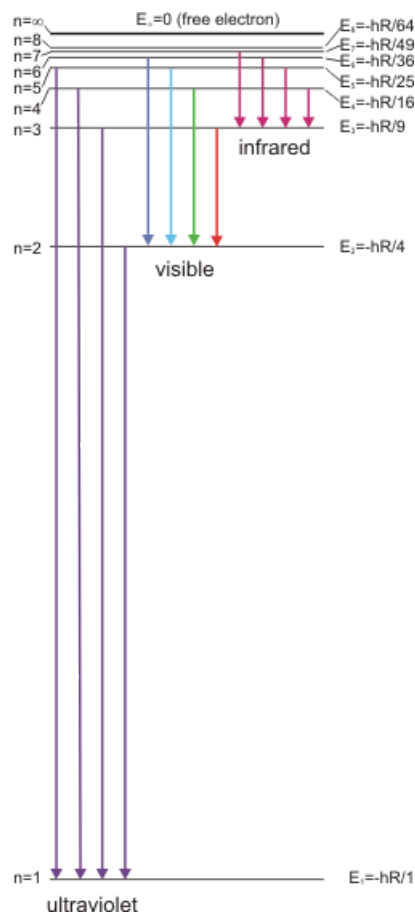


Figure 2.8: Energy Level Diagram for Hydrogen

2.3-5. Color

In a gas discharge tube, a high energy electron collides with an atom and transfers some of its energy to an electron in the atom, exciting the electron into a higher energy level (energy is absorbed). However, electrons always seek the lowest energy level, so the excited electron soon returns to a lower energy level. When it does so, it must give up all or some of the energy that it absorbed initially. Many of the electrons that are excited in this manner give up their energy by emitting photons. Only a fraction of the emitted photons fall in the visible region of the spectrum, but they are the ones that produce the glow in the tube.

Light is a form of energy that results from changes that occur during atomic and molecular processes, and its frequency depends upon the type of process. For example, molecules absorb microwave radiation when they rotate, and they absorb infrared radiation when their atoms vibrate back and forth against their bonds. Visible light originates in electronic transitions; all color is the result of these transitions. A red shirt appears red because it reflects the red portion of white light and absorbs the green portion. The fabric of the shirt contains dye molecules that have electrons that absorb green light when they undergo electronic transitions between energy levels. The levels, however, are not separated by an energy equal to the energy of red photons, so the red photons are reflected and not absorbed. Our eyes perceive the reflected red photons but not the green ones that are absorbed by the shirt.

2.4 Quantum Theory

Introduction

The theory that explains blackbody radiation, the photoelectric effect, and line spectra is called quantum theory. Quantum theory completely changed the way we think about matter. This lesson completes our study of the evolution of chemical theory from Lavoisier's introduction of elements and compounds to where it is today.

Objectives

- Explain what is meant by *electron density* and why it is used instead of electron position.

2.4-1. Vibrating Strings

The reason behind quantization was the cause of much discussion, and the answer was finally presented by a graduate student in his Ph.D. thesis. Louis deBroglie⁴ recognized a similarity between the behavior of electrons and that of a vibrating string!

Plucking a string of length L that is tied at both ends produces standing waves as shown in Figure 2.9. Since the string is tied down at each end, there must be an integral number of half-wavelengths in the distance L , i.e., the wavelength of each wave (λ) must obey the relationship $L = n \times (\lambda/2)$ or $\lambda = 2L/n$. The various values of the integer n define the harmonics. Note that $L = 0$ (no string) when $n = 0$, so n cannot be zero. This is analogous to the Bohr model where the n quantum number is a positive, nonzero integer.

The points where the waves have zero amplitude are called **nodes** (indicated by arrows for $n = 2$ and $n = 3$). Each wave has $(n - 1)$ nodes, not counting the two ends.

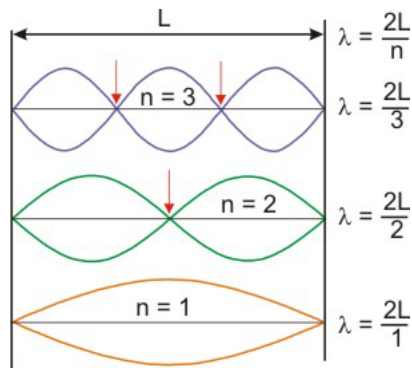


Figure 2.9: Standing Waves in a Vibrating String If the length of the string is L , then the wavelength of each wave is $\lambda = 2L/n$, where n is a nonzero integer. The number of nodes, points of zero amplitude, present in each wave as dictated by the red arrows is $n - 1$.

2.4-2. Quantum Theory

Electrons can behave as either particles or waves.

deBroglie concluded that the quantization proposed by Bohr resulted because the electron has wave properties. His hypothesis was later confirmed by experiment. Like light, the electron had to be treated as both a particle and a wave! The hypothesis seemed crazy, even Einstein said so. “But, it is really sound!” Einstein admitted. The electron’s behavior is dictated by the experiment. Thus, Thomson and Millikan measured the charge and mass of a particle because their experiments were setup to detect particles, but other experiments demonstrated that electrons are diffracted just like waves.

The fact that the electron has wave properties imparts some uncertainty about its position and trajectory. Thus, we cannot predict exactly where an electron will be at any given time. Instead, we must talk about the probability that the electron will be found in some region of space, and the larger the region of space, the greater the probability that the electron will be found in it. As a result, we usually refer to regions of *electron density* rather than the position of the electrons. The electron density is high in regions where the probability of finding an electron is high.

Visit the IBM site⁵ to see the effect of electrons interfering with each other in some great STM (scanning tunneling microscopy) images.

⁴<http://www-groups.dcs.st-and.ac.uk/~history/Mathematicians/Broglie.html>

⁵<http://www.almaden.ibm.com/vis/stm/stm.html>

2.5 The Quantum Numbers

Introduction

Electrons must be treated like waves in modern quantum theory, and their full description requires four numbers called quantum numbers. In this section, we identify the four quantum numbers for an electron in an atom and explain the relationships between them.

Objectives

- State the restrictions on each of the quantum numbers.
- Indicate the information available from each quantum number.
- Differentiate between an acceptable and unacceptable sets of quantum numbers and correct unacceptable sets.
- Give the letter used to describe each value of the l quantum number.
- Indicate the relative energies of several sublevels given their n and l quantum numbers.

2.5-1. Quantum Numbers and Orbital Energy Video

A video or simulation is available online.

2.5-2. Introduction

Four quantum numbers are required for the complete description of an electron in an atom.

In 1926, Erwin Schrödinger applied the wave equation of a vibrating string to the electron. Solving the wave equation produces mathematical functions called *wave functions*. A wave function contains all of the pertinent information about the electron in the atom. Thus, an electron is treated mathematically like a vibrating string in modern quantum theory, and its full description requires four *quantum numbers*. With these four quantum numbers and their relationships to one another, a convincing picture of the electronic structure of the atom can be drawn, one that explains both atomic spectra and chemical periodicity.

The four quantum numbers required to fully characterize an electron are: n , l , m_l , and m_s . The relationships between the quantum number, which are discussed below, are responsible for the periodicity of the chemical properties of the elements.

2.5-3. n Quantum Number

The n quantum number dictates the energy level of the electron.

n is the **principal quantum number**.

- The *principal quantum number* dictates the energy *level* of the electron, so it is the *primary*, but not sole indicator of the electron's energy.
- n also indicates the *average* distance from the nucleus. On the average, electrons with high n quantum numbers are farther from the nucleus than those with lower n quantum numbers.
- Restrictions on n : n must be a nonzero, positive integer, i.e., $n = 1, 2, 3, \dots, \infty$.

2.5-4. l Quantum Number

The n and l quantum numbers determine an electron's sublevel, which determines the electron's energy.

l is the **angular momentum quantum number**.

- n and l define the *sublevel*. The energy of the electron depends upon the sublevel it occupies.
- Restrictions on l : l is an integer such that $0 \leq l < n$ in any sublevel.
- There are n sublevels in each level. For example, if $n = 3$ level, then l can be 0, 1, or 2 for a total of three sublevels.

The following letters are normally used in lieu of the l quantum number to indicate a sublevel.

l quantum number	letter designation
0	s
1	p
2	d
3	f

Note: the letters are derived from the appearance of the lines in an atomic line spectrum: s = sharp, p = principle, d = diffuse, f = fundamental. Sublevels with $l > 3$ are labeled in order as g, h, i,

2.5-5. m_l Quantum Number

n , l , and m_l specify the electron's orbital.

m_l is the **magnetic orbital quantum number**.

- n , l , and m_l specify the **orbital**.
- l and m_l dictate the shape of the orbital, while n defines its size.
- Restrictions: the allowed values of m_l depend upon the sublevel. $-l \leq m_l \leq +l$, so there are $2l + 1$ orbitals in a sublevel.

Electrons reside in orbitals that are characterized by a unique set of three quantum numbers (n , l and m_l). The restrictions on the quantum numbers dictate the number of orbitals in a sublevel and the number of sublevels in a level. Consider the case of the $n = 3$ level shown in Figure 2.10, where each line represents one orbital. Because $n = 3$, there are three sublevels: $l = 0, 1$, and 2 , which correspond to the 3s, 3p and 3d sublevels, respectively. In an $l = 0$ sublevel, there can be only one value of m_l and, therefore, only one orbital ($m_l = 0$). This is the 3s orbital. In an $l = 1$ sublevel, there are three allowed values of m_l ($-1, 0, +1$) and, consequently, three orbitals. These three orbitals are the 3p orbitals. In the $l = 2$ sublevel, $m_l = -2, -1, 0, +1$, and $+2$ for the five orbitals in the 3d sublevel. Thus, in the $n = 3$ level, there are three sublevels and nine orbitals.

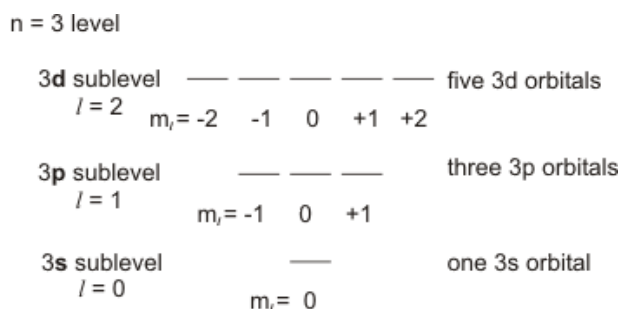


Figure 2.10: Sublevels and Orbitals of the $n = 3$ Level

2.5-6. m_s Quantum Number

m_s determines the electron's spin. All magnetic fields are due to spin.

m_s is the **spin quantum number** that has values of $+1/2$ and $-1/2$ only. Electron spin is responsible for magnetic fields. Although the "spin" property of an electron is a relativistic one, it is common to represent it with a classical analog because a charge moving in a circle does generate a magnetic field. Indeed, the circular motion of electrons is the basis for electromagnets.

A video or simulation is available online.

The wave equation developed by Schrödinger required only the n , l and m_l quantum numbers, but many details of the emission spectra of the atoms could not be explained using only this set of quantum numbers. In addition, silver

atoms that are passed through a magnetic field are divided into two beams. All of these problems could be explained only if the electron had magnetic properties, which required a new quantum number, the electron spin. Electron spin is a quantum mechanical effect that is as much a property of the electron as is its charge. However, a simple macroscopic analogy is often used to describe this quantum mechanical effect. In the analogy (Figure 2.11), electron spin results from the rotation of the electron about its axis (analogous to the 24 hour rotation of the Earth about its axis). The rate of rotation is the same for all electrons, but there are two different directions of rotation, which are distinguished by the spin quantum number, m_s , which has only two possible values: $m_s = +1/2$ and $m_s = -1/2$. All magnetic properties are attributed to electron spin, so it is often represented as the spin of the electron about its own axis in a clockwise ($m_s = +1/2$) or counterclockwise ($m_s = -1/2$) direction because a magnetic field is produced by a charge moving in a circular path. Thus, the ‘spinning charge’ can be thought to generate a magnetic field as indicated by the arrows in Figure 2.11. The arrow representing the magnetic field is often used to represent the m_s quantum number of the electron. An up arrow (‘up spin’) is used to indicate an electron with $m_s = +1/2$ and a down arrow (‘down spin’) indicates an electron with $m_s = -1/2$.

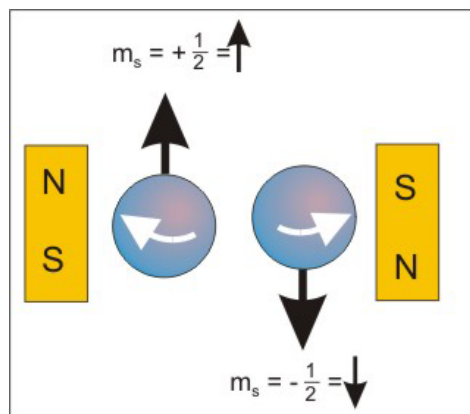


Figure 2.11 The two values of m_s are represented with up or down arrows.

2.5-7. Energy Levels and Quantum Numbers

Sublevels are named by giving the n quantum number followed by the letter that designates the l quantum number.

Sublevels are named by giving the n quantum number followed by the letter that designates the l quantum number. Thus, the sublevel with $n = 3$ and $l = 2$ is referred to as the 3d sublevel.

The relative energies of the sublevels can be determined from the following:

- They increase with the value of $(n + l)$ for the sublevel.
- The energies of sublevels with the same value of $(n + l)$ increase with increasing n .

2.5-8. Quantum Number Exercise

EXERCISE 2.4:

What are the n and l quantum numbers for a 6f electron?

$n =$ _____

$l =$ _____

What is the designation of each of the following sublevels?

$n = 3, l = 2$ _____

$n = 5, l = 1$ _____

$n = 6, l = 3$ _____

$n = 4, l = 0$ _____

How many sublevels are in an $n = 4$ level?

Which sublevel is at lower energy?

4s

3d

Which sublevel is at lower energy?

4p

3d

2.5-9. Quantum Number Restrictions Exercise

EXERCISE 2.5:

The following sets of quantum numbers are not valid but can be made so by correcting one value. Identify the invalid quantum number as n , l , m_l , or m_s in each and supply an acceptable value. If there is more than one acceptable value enter the lowest, positive value or zero.

$n = 3, l = 3, m_l = -3, m_s = +1/2$

invalid number:

n

l

m_l

m_s

acceptable value _____

$n = 75, l = 74, m_l = 0, m_s = 0$

invalid quantum number:

n

l

m_l

m_s

acceptable value _____

$n = 6, l = -5, m_l = -5, m_s = -1/2$

invalid quantum number:

n

l

m_l

m_s

acceptable value _____

$n = 2, l = 0, m_l = 2, m_s = +1/2$

invalid quantum number:

n

l

m_l

m_s

acceptable value _____

2.6 Orbital Shapes and Sizes

Introduction

Orbitals are at the heart of chemistry because it is the interaction between orbitals that produces chemical bonds. Mathematically, an orbital is a wave function with specified values for n , l , and m_l . Like other functions, they can be positive or negative, and the sign of the orbital will be important when we combine them to produce molecular orbitals in Chapter 6. In this section, we consider the shapes of only the s and p orbitals because they are the only orbital types that will be used in the next several chapters.

Objectives

- Draw s orbitals.
- Draw p orbitals and define nodal planes.

2.6-1. s Orbitals

s orbitals are spherical and positive everywhere.

n , l , and m_l designate an orbital. Orbital pictures are used to represent regions where the electrons are most likely to be found (i.e., occupied orbitals are regions of high electron density). Chemical bonding results from the interaction of orbitals and the electrons in them. l and m_l dictate the shape and orientation of the orbital, respectively, and n dictates its size.

l is zero for an s orbital, so m_l must also be zero. Therefore, there can be only one orbital (an s orbital) in an s sublevel. s orbitals are all spherical (the charge is distributed equally in all directions). The sign of an s wave function is always positive. s orbitals in different levels differ only in size and energy.

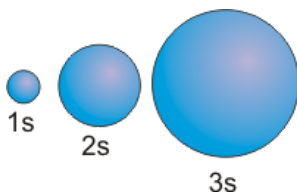


Figure 2.12: s Orbitals The relative sizes of the 1s, 2s, and 3s orbitals of an atom

2.6-2. p Orbitals

p orbitals each contain a nodal plane.

$l = 1$ for p orbitals. There are three values of m_l ($-1, 0, +1$), so there are three orbitals in a p sublevel. The three p orbitals are perpendicular to one another and are referred to as the p_x , p_y , and p_z orbitals. The electron density in each p orbital lies along one of the cartesian axes, but each orbital contains a **nodal plane**, a plane of zero electron density that passes through the nucleus of the atom. The nodal plane is shown as a gray rectangle in Figure 2.13a. In general, the number of nodal planes in an orbital is equal to its l quantum number. $l = 1$ for p orbitals, so they each have one nodal plane.

The function that describes a p orbital is positive in one lobe, zero at the nodal plane, and negative in the other lobe. The fact that the sign of the orbital functions is different in the two lobes will be important in our discussion of bonding, and this point is often emphasized by the shading of the two lobes. We use blue and red to distinguish between the two. Blue will be used to identify lobes where the function is positive and red will be used for lobes in which the function is negative.

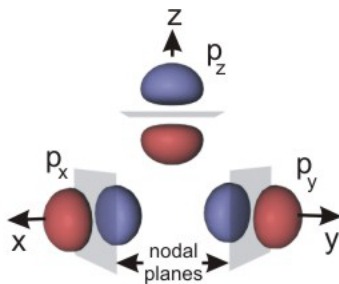


Figure 2.13a: p Orbitals: True Representation

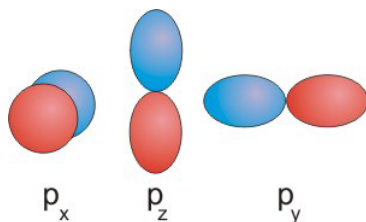


Figure 2.13b: p Orbitals: Common “Figure 8” Representation

2.6-3. d Orbitals

d orbitals each contain two nodal planes.

There are five possible values of m_l in an $l = 2$ sublevel ($-2, -1, 0, +1, +2$), so there are five d orbitals. Figure 2.14 shows a representation of these orbitals. The d_{z^2} (or simply z^2) orbital is directed along the z -axis, but there is a donut shaped region of electron density in the xy -plane. The $x^2 - y^2$ orbital is directed along both the x - and the y -axes in both the positive and negative directions. Much of the d_{xz} (xz) electron cloud lies in the xz -plane 45° from either axis. The shapes of the d_{yz} (yz) and d_{xy} (xy) are identical to that of the d_{xz} , only the labels of the axes change.

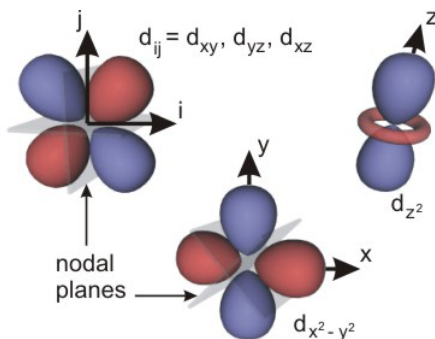


Figure 2.14: d Orbitals

2.7 Electron Configurations

Introduction

The number of electrons in each sublevel is given by the electron configuration of an atom. Electron configurations, the topic of this section, will help us predict the bonding properties of an atom.

Objectives

- Write an electron configuration from a sublevel population.
- Use the Pauli Exclusion Principle to distinguish between acceptable and unacceptable ways for electrons to occupy an orbital.
- Use Hund's Rule to determine a lowest energy electron configuration of an atom with a partially filled sublevel.
- Determine the lower energy configuration based on the sublevel populations of two different configurations
- Determine whether an arrangement of electrons represents a ground state, an excited state, or is not acceptable.
- Use an energy level diagram and the number of electrons in an atom to write the ground state electron configuration of the atom.
- Determine the number of unpaired electrons in an atom's ground state electron configuration.
- Write electron configurations using the noble gas core abbreviation.
- Write the electron configurations for the two elements in the fourth period that are exceptions to the trend in configurations.

2.7-1. Electron Configurations Video

A video or simulation is available online.

2.7-2. Electron Configurations

An electron configuration specifies the occupied sublevels and the number of electrons in each.

The sublevel in which an electron resides can be determined because the energy of the electron can be determined. However, the orbital that contains the electron cannot be determined because the orbitals in a sublevel all have the same energy and differ only in their orientation. Consequently, the electronic structure of an atom is normally given as a list of the occupied sublevels and the number of electrons in each sublevel. This list is called the atom's **electron configuration**. The notation used for each sublevel is $n l^p$

- n is the n quantum number.
- l is the l quantum number of the sublevel expressed as a letter (s, p, d, ...).
- p is the sublevel population (i.e., the number of electrons in the sublevel).

For example, an electron configuration of $1s^2 2s^2 2p^3$ indicates that there are two electrons in the 1s sublevel, two electrons in the 2s sublevel, and three electrons in the 2p sublevel. The superscripts give the number of electrons in each sublevel, so the **sum of all of the superscripts in an electron configuration must equal the number of electrons in the atom or ion**. Therefore, the above configuration is for the atom that has seven electrons ($2 + 2 + 3$), which is the nitrogen atom.

2.7-3. Pauli Exclusion Principle

No orbital can have more than one electron of a given spin, so no orbital can have more than two electrons.

Pauli Exclusion Principle states that no two electrons in an atom can have the same set of quantum numbers.

Electrons in the same orbital have the same values of n , l , and m_l . Thus, all of the electrons in an orbital must have different m_s quantum numbers. The spin quantum number can be only $+1/2$ or $-1/2$, so the Pauli Exclusion Principle dictates that **an orbital can accommodate a maximum of two electrons, one with spin up ($m_s = +1/2$) and one with spin down ($m_s = -1/2$)**.

Since, the two electrons in an orbital have opposite spins, they are said to be **paired**. An electron that occupies an orbital alone is said to be **unpaired**. Similarly, an orbital with two electrons is full, while an orbital with one electron is said to be **half-filled**.

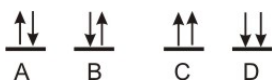


Figure 2.15: Pauli Exclusion Principle A and B are acceptable, but C and D are not because they violate the Pauli Exclusion Principle.

2.7-4. Hund's Rule

The lowest energy arrangement of electrons in an unfilled sublevel is the one that maximizes the number of electrons with identical spin.

Hund's Rule states that the lowest energy arrangement of electrons in an unfilled sublevel is the one that maximizes the number of electrons with identical spin. Hund's Rule is only an aid for determining the lowest energy arrangement of electrons in partially filled sublevels with more than one orbital (p, d, and f). *Arrangements that violate Hund's Rule can be acceptable, but they cannot be the lowest energy arrangement.* Hund's Rule guarantees that the number of unpaired electrons in a sublevel is maximized in atoms.

Note that the direction of the spin does not matter, but maximizing the number with identical spins does. Thus, the lowest energy arrangement of three electrons in a p sublevel consists of one electron in each orbital and all electron spins the same (all up or all down).

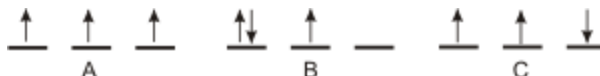


Figure 2.16: Hund's Rule A is the lowest energy configuration because it obeys Hund's Rule. The energies of B and C are greater than that of A because the three spins are not the same. B and C are excited states.

2.7-5. Lowest Energy Configurations

Electrons occupy the unfilled orbitals of lowest energy (i.e., the sublevels with the lowest value of $n + l$). Remember that the energies of sublevels with the same value of $(n + l)$ increase in order of increasing n . Also recall that l cannot be greater than $(n - 1)$. The order of sublevels in increasing energy through $(n + l) = 7$ is given below.

order	$n + l$	n	l	sublevel
1	1	1	0	1s
2	2	2	0	2s
3	3	2	1	2p
4	3	3	0	3s
5	4	3	1	3p
6	4	4	0	4s
7	5	3	2	3d
8	5	4	1	4p
9	5	5	0	5s
10	6	4	2	4d
11	6	5	1	5p
12	6	6	0	6s
13	7	4	3	4f
14	7	5	2	5d
15	7	6	1	6p
16	7	7	0	7s

2.7-6. Sublevel Energy Diagram

Orbital energies increase with $n + l$. Orbitals with the same value of $n + l$ increase in order of n .

We constructed an energy level diagram for the first 19 orbitals in the Quantum Numbers and Orbital Energy Video. It shows the relative energies (increasing $n + l$) of the sublevels for an atom and the diagram and it is reproduced below. Recall that each line corresponds to an orbital (n , l , and m_l quantum numbers), so two electrons (one spin up and one spin down) can be added to each line.

The Pauli Exclusion Principle states that each orbital can house a maximum of two electrons, so a maximum of 38 electrons could occupy the 19 orbitals represented in Figure 2.17.

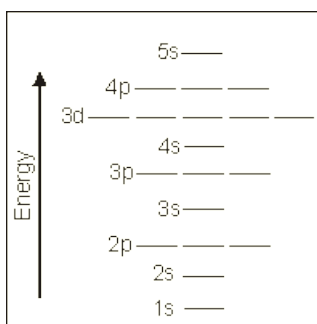


Figure 2.17: Atomic Orbitals in Order of Increasing Energy

2.7-7. Ground States

In the ground state configuration, there can be no unfilled orbitals lower in energy than the highest energy electron.

The electrons in an atom strive toward the lowest energy arrangement that is consistent with the Pauli Exclusion Principle. Such an arrangement is called the **ground state** configuration of the atom. The ground state configuration is the one in which

- 1 the Pauli Exclusion Principle is obeyed.

- 2 the occupied sublevels are those at lowest energy.
- 3 Hund's Rule is obeyed.

Configurations that do not obey the Pauli Exclusion Principle are not acceptable configurations. Those that obey the Pauli Exclusion Principle but not points '2' and/or '3' are acceptable, but they are not ground state configurations. They represent configurations with energies greater than that of the ground state. These high-energy configurations are called **excited state** configurations. Thus, there are many acceptable electron configurations for an atom, but only one represents its ground state; all others are excited state configurations. An atom will be found in its ground state under normal conditions, so when the electron configuration of an atom is written it is understood to be the ground state configuration. However, atoms can be excited from the ground state into one of the excited states with an input of energy.

2.7-8. Unpaired Electrons

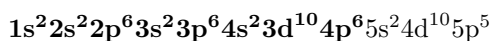
The number of unpaired electrons in a sublevel is maximized by Hund's Rule.

The electrons in the ground state of an atom occupy the lowest energy sublevels consistent with the Pauli Exclusion Principle and Hund's Rule. This allows us to determine two important properties of an atom.

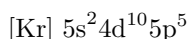
- 1 **Ground state electron configuration:** the listing of the occupied sublevels and their populations
- 2 **Unpaired electrons:** Unpaired electrons exist in unfilled sublevels and their number is maximized by Hund's Rule. (As we will see in Chapter 3, the number of unpaired electrons is an important characteristic of the atom because it dictates the atom's magnetic properties.)

2.7-9. Using Noble Gas Cores in Electron Configurations

The electron configurations of the atoms become unwieldy as the number of electrons in the atom increases. For example, iodine's electron configuration is



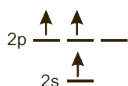
and bismuth has 30 more electrons than iodine. These lengthy configurations can be shortened considerably by using the fact that the electron configuration of every element after a noble gas consists of that noble gas configuration plus some other entries. In the configuration of iodine above, the portion in bold is the electron configuration of Kr, which is abbreviated as [Kr]. Thus, the electron configuration of iodine can be shortened substantially to the following.



2.7-10. Electron Configuration Exercises

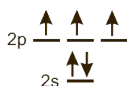
EXERCISE 2.6:

Write the electron configuration of each of the following diagrams. Also indicate whether the configuration is ground state or an excited state configuration.



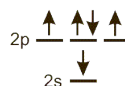
configuration:

ground state
excited state



configuration:

ground state
excited state



configuration:

ground state
excited state

2.7-11. Two Exceptions

Chromium and copper are the only two exceptions we deal with.

The energy difference between the s and d sublevels within a level is relatively small, and they get smaller as n increases. The introduction of f sublevels decreases the energy difference between sublevels even more. Such small differences lead to exceptions to our predicted configurations for elements filling d and f blocks as even minor changes can cause electrons to enter a higher energy sublevel. For this reason, we consider only the first row of the transition elements and none of the inner transition elements. There are two exceptions even in the 4th period that result from the fact that the spherical charge distribution accompanying filled and half-filled sublevels lowers the energies of these configurations. Indeed, the amount by which the energy is lowered is greater than the separation between the 4s and 3d sublevels, so a single electron is promoted from the 4s to the 3d to attain these configurations. The two exceptions in which this occurs are:

- 1 **Chromium** promotes a 4s electron to attain an $[\text{Ar}] 4s^1 3d^5$, which has a half-filled 3d sublevel.
- 2 **Copper** promotes a 4s electron to attain an $[\text{Ar}] 4s^1 3d^{10}$, which has a filled 3d sublevel.

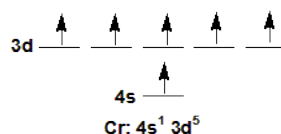


Figure 2.18 Cr promotes a 4s electron to attain a half-filled 3d sublevel.

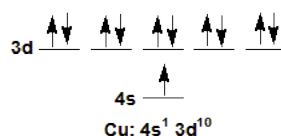


Figure 2.19 Cu promotes a 4s electron to attain a filled 3d sublevel.

2.7-12. Energy Level Exercise

EXERCISE 2.7:

Extend the energy level diagram for the sublevels to include $n + l = 6$ and $n + l = 7$. Place the lowest energy sublevel at the bottom (4d) and the highest energy sublevel at the top (7s). Include the number of orbitals in each.

sublevel	7s	orbitals	_____
sublevel	_____	orbitals	_____
sublevel	_____	orbitals	_____
sublevel	_____	orbitals	_____
sublevel	_____	orbitals	_____
sublevel	_____	orbitals	_____
sublevel	4d	orbitals	_____

2.7-13. Shorthand Notation Exercise

EXERCISE 2.8:

Use the energy level diagram for the sublevels through $n + l = 5$ in Figure 2.17 and the levels for $n + l = 6$ and 7 that were determined in the previous exercise to determine sublevel populations for the ground states of the following. Then use the noble gas core shorthand to write their electron configurations. Place a space after the noble gas and between each sublevel. The sublevel energies continue from those.

Rb _____

Sn _____

Bi _____

2.7-14. Hund's Rule Exercise

EXERCISE 2.9:

Which arrangement of d electrons has the lowest energy in each case?



A
B
C
D

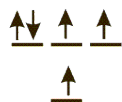


A
B
C

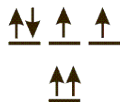
2.7-15. Identifying States Exercise

EXERCISE 2.10:

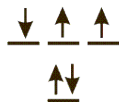
Indicate whether each of the following represents a ground state, an excited state, or are unacceptable configuration. Assume that all sublevels at lower energy are filled.



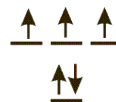
ground state
excited state
not acceptable



ground state
excited state
not acceptable



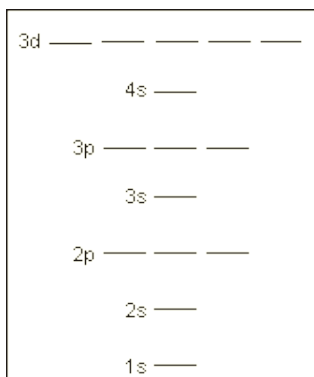
ground state
excited state
not acceptable



ground state
excited state
not acceptable

2.7-16. Unpaired Electrons Exercise

EXERCISE 2.11:



C (6 electrons):

configuration _____

unpaired electrons _____

Mg (12 electrons):

configuration _____

unpaired electrons _____

Fe (26 electrons):

configuration _____

unpaired electrons _____

2.8 Quantum Theory and The Periodic Table

Introduction

Like other atomic properties, the electron configurations of the atoms are periodic. This periodicity allows us to determine the electron configuration of an atom from the atom's position in the periodic table.

Objectives

- Write the electron configuration of an atom from its placement in the periodic table.

2.8-1. Periodicity of Electron Configurations Video

A video or simulation is available online.

2.8-2. Electron Configurations and Periodicity

The sublevels fill in the following order (left to right then down).

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

Each column represents the same type of sublevel (s, p, or d). The number of electrons required to fill each of these sublevels is

- 1** s sublevel: 2 electrons.
- 2** p sublevel: 6 electrons.
- 3** d sublevel: 10 electrons.

Changing the width of each column to reflect the number of electrons that are required to fill each sublevel, we obtain the following view.

[illegible]

The above table has exactly the same form as the periodic table. If you understand this periodicity, you can determine the electron configuration of an atom from its position in the periodic table.

2.8-3. Periodic Table and Sublevels

s Block

The $n = 1$ level contains only one s sublevel. Thus, H and He are $1s^1$ and $1s^2$, respectively. However, their positions in the periodic table are normally not with the other elements of the s block. Hydrogen is often shown in the middle of the periodic table for reasons that will be explained in Chapter 4, and He is at the top of the Group 8A elements because it is a noble gas. The rest of the s block elements are those in Groups 1A and 2A. The n quantum number of the level to which the outermost sublevel belongs is given by the row number. Thus, **the electron configurations of the outermost sublevel** for the Group 1A and 2A elements are the following.

1A	2A
ns^1	ns^2

p Block

The elements of Groups 3A through 8A are filling a p sublevel. The n quantum number of the level to which the outermost sublevel belongs is given by the row number. Thus, the **electron configurations of the outermost sublevel** for the Group 3A through 8A elements have the following form.

3A	4A	5A	6A	7A	8A
np^1	np^2	np^3	np^4	np^5	np^6

d Block

The elements of Groups 3B through 2B are filling a d sublevel. The n quantum number of the level to which the d sublevel belongs equals the row number $- 1$. Thus, elements scandium ($Z = 21$) through zinc ($Z = 30$) are filling the 3d sublevel, while yttrium ($Z = 39$) through cadmium ($Z = 48$) are filling the 4d sublevel.

Figure 2.20: s, p, d, and f Blocks in the Periodic Table

Practice using the periodic table to predict the electron configuration of an atom. Check your answer by clicking on the element in the periodic table available online.

EXERCISE 2.12:

Use the periodic table to help you write electron configurations for the following atoms. Use the Noble gas core abbreviation.

	1A	2A											3A	4A	5A	6A	7A	8A		
	s block												p block							
D	1		d block																	
1	H	2	3B	4B	5B	6B	7B	8B			1B	2B	1	2	3	4	5	He		
2	Li	Be											B	C	N	O	F	Ne		
3	Na	Mg	1	2	3	4	5	6	7	8	9	10	Al	Si	P	S	Cl	Ar		
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt											
											f block									
	1	2	3	4	5	6	7	8	9	10	11	12	13	14						
	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu						
	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr						

Sc _____ N _____ Cu _____
Bi _____ K _____ Co _____

Links to view either the end-of-chapter exercises or the solutions to the odd exercises are available in the HTML version of the chapter.