



College Chemistry

A Comprehensive Set of Imperfect Notes

Daniel Torres



January 21, 2024 (3:50pm)

1 IA

1	H	Hydrogen
3	Li	Lithium
2	Be	Boron
5	Mg	Magnesium
11	Na	Sodium
19	K	Calcium
37	Rb	Rubidium
55	Cs	Cesium
87	Fr	Francium

Periodic Table of Chemical Elements

18 VIIA

z mass Symbol	1 IA	2 IA	3 IA	4 IA	5 IA	6 IA	7 IA	8 IA	9 IA	10 IA	11 IA	12 IA	13 IA	14 IA	15 IA	16 IA	17 IA
1	H	Hydrogen															
3	Li	Lithium															
2	Be	Boron															
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TO THE READER

First and foremost, I genuinely care about the progress of every one of my students and I want to see you all succeed. This is why I decided to write this manuscript. This set of lecture notes was designed with a focus on the student—with a focus on you. It introduces the basic concepts of college chemistry in a way that a student of any level can hopefully understand. Some of the chapters included in this guide can be challenging. Success is not an accident. Only with hard work, patience, and perseverance, you will be able to achieve what you want. I hope to encourage you not only to successfully pass this class. More importantly, I hope to inspire you to see that you can do this.

College chemistry is not an easy subject. You may experience frustration due to the terminology or the math content. This guide is developed in chapters and sections to break down the very basics of chemistry concepts. One of my main goals is to help you solve chemistry problems. Solving problems—not only chemistry problems but problems of any kind—is an extremely useful skill in life. Chemists approach the solving of problems in a very specific way. They use critical thinking and previous knowledge to find solutions based on the information presented. As you study this set of lectures, I encourage you to read the different sections of a chapter, highlight the main ideas and find keywords that represent new concepts. Numerous examples are presented in the chapters with the full solution. A lot of examples are also presented without the worked solution, just including the answer. Plenty of end of the chapter problems is further included. After you read the content of a chapter I highly encourage you to work on the end of the chapter problems. As with any skill, practice makes perfect.

I used numerous tools in this guide to help you focus on the most relevant content. For example, when the numerical problems get too complex, an *analyze the problem box* is included to help you identify what is given and what is asked in the problem.

This set of lectures resonates with the open textbook movement that is taking over CUNY as well as SUNY. Education is expensive and you as a student often rely on textbooks to learn. These valuable educational resources are often used for a very limited period and tossed or returned when a class has finished. The open textbook movement aims to alleviate the cost of education by relying on resources that are free for both the students and the educators. Still, these sources are imperfect and not as curated as textbooks, and this is the price to pay. I warn you this set of the lecture is indeed imperfect, hence its title. Yet, it is the result of many hours of work—indeed months of work. Your role is key. I encourage you first to be understanding and patient, and then to contribute to the

development of this guide. With your input, we can make this guide a better educational resource. Mind that this guide was written by an educator and as such, it sometimes uses terms and a way of thinking that corresponds to the educators' point of view.

This set of lectures does not intend to replace any textbook. Indeed, there are many high-quality textbooks in the literature that I recommend. For College Chemistry:

- Chemical Principles: The Quest for Insight by Peter Atkins et al.
 - Chemistry: The Central Science by Theodore E. Brown et al.
 - Chemistry by Steven S. Zumdahl et al.
 - Chemistry: The Molecular Nature of Matter and Change by Martin Silberberg et al.
 - Chemistry by Raymond Chang et al.
 - Chemistry: Atoms First by OpenStax
- For GOB Chemistry:
- General, Organic, and Biological Chemistry: Structures of Life by Karen C. Timberlake et al.

With the help of the textbooks above you can certainly expand and complement the information presented in this guide.

This guide was fully coded in *LATeX* from the cover or the periodic table to the molecular orbital diagrams or the solid representations. Chemistry is a microscopic science not accessible to the naked eye. Visuals play a very important role in chemistry education. Visuals—in the form of images or diagrams—help make chemistry more apparent to the viewer. One of the weak points of many open education chemistry guides is the visuals. They tend to be simplistic with low quality. This guide extensively relies on images and diagrams and uses the *Tikz* software package and other open-source tools to freshly generate diagrams everytime the book is compiled. All other images used here are open-source images.

The work of chemists is certainly challenging, but also exciting and rewarding. Chemists produce everything from plastics and paints to pharmaceuticals, foods, flavors, fragrances, detergents, and cosmetics. Chemistry students are well-prepared for medical, veterinarian, dentistry, optometry, or pharmacy school. I hope you enjoy this guide and more importantly I wish you success in your career.



Daniel Torres
Brooklyn



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Ch. 1. Measurements

MEASURING is an important part of our everyday lives, and very probably you took several measurements today. You might now be sipping a cup of coffee, or perhaps you checked the outside temperature on a street thermometer. You might be planning to bake a cake and need to use a scale and a cup to measure the flour and sugar. A cup, a thermometer, or a scale are measuring devices. It is critical to know how to accurately measure properties and, more importantly, how to transform measurements using prefixes and unit conversions. By learning how to measure and perform operations with units, you will gain experience performing basic chemistry calculations.

1.1 Math skills

There are a few math skills that are critical to be able to carry out chemistry problems. Those skills entail operating with numbers, converting numbers into scientific notation, solving basic equations, and interpreting graphs.

Place values We can identify the place value in any number for all its digits. The place values are named based on the location concerning the decimal place. For digits to the left of the decimal place, the place values are called the ones, the tens, the hundreds, and the thousands. For example, in the value 3456s, the number 3 is the thousands place, the number 4 is the hundreds place, 5 is the tens place and 6 is the one's place. For digits to the right of the decimal place, the place values are called the tenths, the hundredths, and the thousandths, mind the suffix *ths*. For example, in the value 3.456Kg, the number 3 is the one place, the number 4 is the tenth place, 5 is the hundredth place and 6 is the thousandth place.

Basic algebra Positive numbers are larger than zero whereas negative numbers are smaller than zero. Negative numbers are written with a negative (-) sign. The multiplication or division of two positive or two negative numbers always gives a positive result, whereas the multiplication or division of a positive and a negative number always gives a negative result. When we add two positive numbers the results are always positive, whereas when we add two negative numbers the results are always negative. When positive and negative numbers are added, the results come from subtracting the smallest number from the largest number while keeping the sign of the larger number. In a calculator, there is a key $\boxed{-}$ (sometimes shown as $\boxed{+/-}$) used to switch the sign of a number.



Solving equations When solving the equation below for x ,

$$3x - 4 = 8$$

some basic algebra rules apply:

- 1 **Step one:** Place all like terms in one side
 - 2 **Step two:** Isolate the variable you want to calculate
 - 3 **Step three:** Check the answer

When placing like terms on the same side, you can eliminate terms by adding, subtracting, multiplying, or dividing. Make sure you apply those rules on both sides of the equation at the same time. For the example above, we will first eliminate the -4 by subtracting 4 in both sides:

$$3x - 4 + 4 = 8 + 4$$

That gives,

$$3x = 12$$

Now we will remove the 3 by diving by three on both sides:

$$\frac{3x}{3} = \frac{12}{3}$$

Therefore we have

$$x = \frac{12}{3} = 4$$

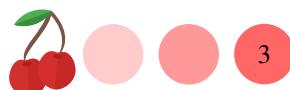
Scientific notation Numbers in science can often be very large or very tiny.

345000g (full notation) 3.45×10^5 g (scientific notation)

To express a number smaller than one (e.g. 0.000134g) in scientific notation, we just need to leave the first digit followed by the decimal point which was moved in this case to the right 4 places, giving 1.34×10^{-4} g as indicated below

0.000134g (full notation) $1.34 \times 10^{-4}\text{g}$ (scientific notation)

You can enter scientific notation numbers in a calculator using a specific key that contains the \times character and the power of ten. For example, the number 1×10^6 should



be typed in a calculator as $1\text{EE} 6$ or $1\text{EXP} 6$ or 1×10^6 , depending on your calculator. For numbers with a negative power of ten, you should use the $(-)$ key (sometimes shown as $(+/-)$) to indicate the sign. For example, the number 1×10^{-5} should be typed in a calculator as $1\text{EE} (-) 5$ or $1\text{EXP} (-) 5$ or $1\times 10^6 (-) 5$, depending on your calculator. The calculator display often can display a scientific notation number differently, based on the calculator brand. Below are three possible scenarios:

$$1.5 \times 10^{-4}$$

$$1.5\text{E}-04$$

$$6.7 \times 10^{-5}$$

$$6.7\text{ -}05$$

$$4.6 \times 10^{-2}$$

$$4.6\text{e-}02$$

You can also convert full notation numbers into scientific notation with a calculator key named SCI often accessible through the second function key.

Sample Problem 1

Convert the following numbers from full to scientific notation or vice versa:

- (a) 7462.97 (b) 0.000234 (c) 0.012

SOLUTION

The answers are 7.46297×10^3 , 2.34×10^{-4} , and 1.2×10^{-2} .

◆ STUDY CHECK

Convert the following numbers from full to scientific notation or vice versa:

- (a) 12000 (b) 0.00076 (c) 45783

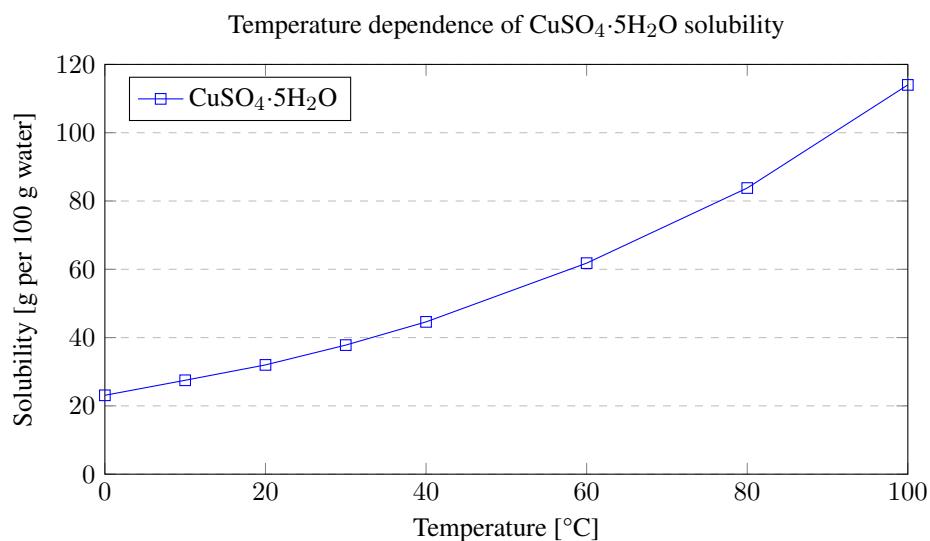


Figure 1.1 A graph plotting the change of solubility of a chemical with temperature.

Interpreting graphs A graph represents data in terms of a relationship between two variables. For example, Figure 1.1 represents the relationship between solubility and temperature. These quantities are plotted along two axes the Y or vertical axis and the X or horizontal axis. The title of the graph indicates what is being represented, and for example, on the graph above we have represented the change of solubility



▼Scales measure mass



© www.wallpaperflare.com

▼Watches are used to measure time



© www.wallpaperflare.com

▼Beakers can carry a liquid volume



© wikipedia

▼Thermometers measure temperature



© PixImg

▼pipets are used in chemistry practice to add an exact volume of liquid



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Section 1.2 ● Units of Measurements and systems of units

of a chemical with temperature. The vertical axis represents solubility given a range between 0 and 120 g/100g of water. The horizontal axis represents temperature with a range between 0 and 100°C. Each point in the graph represents the value of solubility for a given temperature. Based on the graph we can see that solubility slowly increases as temperature increases. We could estimate the value of solubility for any temperature within the range given and for example at a temperature of 50 °C the solubility should be close to 50 g/100g of water.

1.2 Units of Measurements and systems of units

You probably heard the term liter, kilogram, or meter. These are units of measurement. Units can be classified into different *systems of units*. For example, the unit *meter* belongs to a different system than the unit *mile*. In particular, here we will address three main systems: the English System, the Metric System, and the International system. The *Metric System* (MS) is used by scientists throughout the world and is the most common measuring system based on the meter. The English system is mostly used in the US. The *International System of Units* (SI) adopted the metric system in 1960 to provide additional uniformity for units used in the sciences. Table 1.1 summarizes some of the fundamental units for the three systems. This chapter will be mostly based on the SI units. In the following, we will introduce some common units.

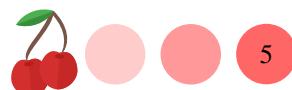
Length What is your height? The length refers to distance and both the metric and SI unit of length is the meter (m). A smaller unit of length would be the centimeter (cm) that is commonly used in chemistry. The most important units of length are meters, inches, and miles.

Mass What is your weight? The mass of an object is a measure of the quantity of material it contains. You may be more familiar with the term weight rather than mass. However, mass and weight are not the same, as weight is a measure of the gravitational pull on an object. It differs depending on your location on the earth—in particular the height of your location. In the metric system, the unit of mass is the gram (g). The SI unit of mass, the kilogram (kg), is used for larger masses such as body weight. A pound, lb, is another unit of mass. The most important units of mass are g, kg, and lb.

Temperature How is the weather today? Is it cold or hot? You use a thermometer to measure temperature and for example assess how hot an object is, or how cold it is outside, or perhaps to determine if you have a fever. Temperature tells us how hot or cold an object is. Temperature can be measured in numerous units such as Celsius (°C), Fahrenheit (°F), or kelvins (K).

Time How long is your commute to work? It might take you hours to go to work, or maybe minutes. You probably think of time as years, days, minutes, or seconds. Of all these units, the International System of units (SI, abbreviated from the French *Système international*) uses seconds (s) to measure time. Still, time can be measured in s, min, or h and during this chapter, we will learn how to convert units of time.

Volume How much milk do you usually buy? Maybe a gallon. Volume is the amount of space that a substance occupies. A liter (L), not a fundamental but a derived SI unit, is commonly used to measure volume. The milliliter (mL) is more convenient for measuring smaller volumes of fluids in hospitals and laboratories. Gallon is still used in everyday life. L, mL, and gallon are units of volume. Units of volume are in general



cubic units, so for example one liter is the same as one dm^3 . We will cover cubit units further in this chapter.

Chemical laboratory work commonly requires the measurement of volume. There are two main types of glassware used to measure volume in a chemistry lab: graduated tools and volumetric tools. Volumetric pipets, flasks, and burets are the most accurate; the glassware makers calibrate these to a high level of accuracy, usually measured in terms of tolerance, which is the uncertainty in a measurement made with the glassware. Class A volumetric glassware has a lower tolerance than Class B; for class A, the tolerance can be as low as 0.08 ml for a 100 ml flask or pipet. Generally, measurements with class A volumetric glassware can be considered reliable to two places after the decimal point. Graduated cylinders, beakers, and Erlenmeyer flasks have less accuracy than volumetric glassware. Graduated cylinders can generally be considered reliable to within 1 percent. Beakers and Erlenmeyer flasks should not be used to measure volume unless you need only a very crude estimate because their accuracy for volume measurements is so poor. They can hold a much larger volume than any of the other types of glassware, however, which makes them useful for mixing solutions.

Concentration Even though we will devote a whole chapter to solutions and concentration, it felt important to introduce here the unit molarity. In chemistry, the unit molarity (M) refers to the concentration of a solution. That is the larger this number, the larger molarity, and the more concentrated a solution will be. In other words, there will be more substance in the solution.

Sample Problem 2

State the type of measurement indicated in each of the following:

- (a) 1ft (foot) (b) 20Kg (c) 3L (d) 300K

SOLUTION

(a) length; (b) mass; (c) volume; (d) temperature;

◆ STUDY CHECK

State the type of measurement indicated in each of the following: (a) 800°F

- (b) 1m^3 (c) 3m (d) 67s

Table 1.1 Different unit systems

Measurements	Metric System	International System (SI)	English System
Length	Meter (m)	Meter (m)	Foot (ft)
Mass	Gram (g)	Kilogram (kg)	Pound (lb)
Time	Second (s)	Second (s)	Second (s)
Temperature	Celsius ($^{\circ}\text{C}$)	Kelvin (K)	Fahrenheit ($^{\circ}\text{F}$)
Volume*	Liter (L)	Cubic meter (m^3)	Gallon (gal)
Ammount of substance	Mole (mol)	Mole (mol)	Mole (mol)
Electric current	Ampere (A)	Ampere (A)	Ampere (A)

*Not a fundamental unit

1.3 Significant Figures

Exact numbers result from counting. For example, think about how many eggs are there in your refrigerator, there might be three and this number is exact. Differently, numbers that



result from a measurement are called measured values and they are subject to uncertainty—in other words error. For example, if you weigh a single egg on a scale depending on the type of scale you used and the person who carries out the measurement, you will measure 70g or 71g, or maybe 70.8g. The mass of an egg is a measured property and hence some of the digits of the measurement are uncertain. The goal of this section is, given a value, to calculate the number of significant figures of a number (we will refer to significant figures as SF, or SFs). Another goal is to estimate significant figures in the calculation to express the result with the right number of digits and significant figures.

Measured numbers *Measured numbers* result from measuring a property such as the weight or length of an object. Those measurements result from using a measuring device such as a scale or a ruler, for example. Imagine we want to measure the length of both objects presented in Figure 1.2. The metric rules presented have a set of marked divisions which determine the number of figures given by the measurement. For example, the ruler on the left has 1cm and 0.1cm divisions, whereas the rule on the right only has 1cm divisions, hence giving fewer figures.

Let us estimate the length of the object on the right. The end of the object on the right is located between 0cm and 1cm, therefore its length is less than 1cm. Still, we can estimate an extra digit by dividing the space between the lines. Still, this last *estimated digit* might differ from person to person. The final measurement would be 0.8cm. However, some people would read the length as 0.7cm whereas others 0.9cm. Let us now estimate the length of the object on the left. The end of the object on the right is located between 3.1cm and 3.2cm, therefore its length is less than 3.2cm. We can estimate an extra digit as well, giving a final measurement of 3.15cm.

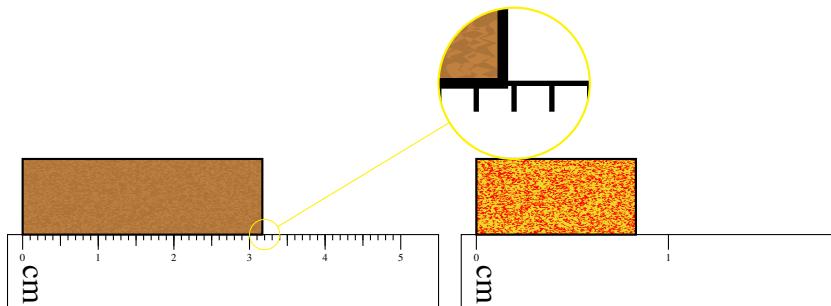


Figure 1.2 Some metric scales with two objects of different lengths. Measurements are (left) 3.15cm (right) and 0.8cm.

Reading menisci Reading a liquid meniscus is similar to reading any measuring scale. There are two types of menisci (see Figure 1.3). A concave meniscus, which is what you normally will see, occurs when the molecules of the liquid are attracted to those of the container. This occurs with water and a glass tube. A convex meniscus occurs when the molecules have a stronger attraction to each other than to the container, as with mercury and glass. If the meniscus is concave, read at the lowest level of the curve. If the meniscus is convex, take your measurement at the highest point of the curve. Let us read the menisci from the image below. Readings are 16.0mL (left), 8.5mL (center left), 18.0mL (center right), and 18.5mL (right).

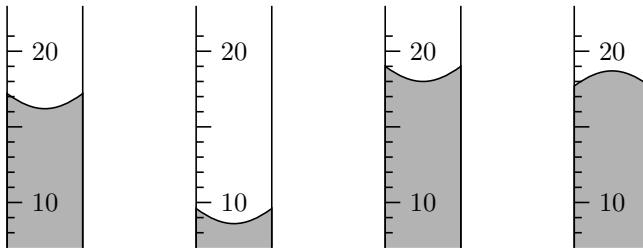


Figure 1.3 Some volumetric measurements in mL are presented in two types of meniscuses. The Left, center-right, and center-left are concave meniscuses, whereas the right image presents a convex meniscus. Readings are 16.0mL (left), 8.5mL (center left), 18.0mL (center right), and 18.5mL (right).

Exact numbers Exact numbers are numbers obtained by counting and not by measuring or obtained by a relationship that compared two units in the same measuring system. For example, the number of students in a class is exact as we need to count to get this number. Similarly, the number of grams in a kilogram, a thousand, is exact as the relationship between kilogram and gram is exact. Exact numbers do not have significant figures and do not limit the number of figures in a calculation.

Significant figures of numbers In general, all numbers different than zero are significant and for example, the number 123 has three significant figures. Similarly, the number 45 has two significant figures. Zeros are also significant except when:

¶ **Exception 1** A zero is not significant when placed at the beginning of a decimal number. For example, the number 0.123 has three significant figures, as the first zero is not significant. Similarly, the number 0.002340 has four significant figures as the first three zeros are not significant but the last zero it is. Mind the rule affects only the zeros at the beginning. A final example:

$$0.032 \text{ (2SF)}$$

¶ **Exception 2** A zero is not significant when used as a placeholder in a number without a decimal point. For example, the number 1000 has only one significant figure, and the number 3400 has two. Let us consider more examples. The number 120 has two significant figures, as according to the second rule the last zero is not significant. Differently, the number 1203 has four significant figures, as the zero in between two numbers is not affected by either the first or the second rule. A final example,

$$3200 \text{ (2SF)}$$

¶ **Exception 3** A zero in a number expressed in scientific notation is significant. For example, the zero in 3.0×10^{-2} is significant, and the number has 2SFs. A final example:

$$3.2020 \times 10^2 \text{ (5SF)}$$

Sample Problem 3

Indicate the number of significant figures in the following numbers: 123, 4567, 1200, 340, 0.001, 0.023 and 0.0405.

SOLUTION

123 has three significant figures, whereas 4567 has four SF. 1200 has only 2SF



as the last two zeros are not significant, and 340 has only 2SF as the last zero is not significant. 0.001 has only one significant figure as the first 3 zeros are not significant and 0.023 has only two SFs. Finally, 0.0405 has threee SFs as the first two zeros are not significant but the zero between 4 and 5 is indeed significant.

❖ STUDY CHECK

Indicate the number of significant figures (SFs) in the following numbers: 4560, 0.123, 1000 and 0.0030.

Significant figures in calculations Two different rules allow you to express the result of calculations with the correct number of figures.

❖ **Rule 1 (+ –)** *For additions or subtractions, the results has the same number of decimal places as the number with the least decimal places in the calculation.* For example:

$$34.3451 + 34.5 = 68.8 \text{ (+ - less decimals)}$$

If you add $34.3451 + 34.5$ you will obtain 68.8451, however, as 34.3451 has four decimal places (4DP) and 34.5 has one decimal place (1DP), the result of adding both numbers will have to have only one decimal place, therefore 68.8451 needs to be rounded to 68.8 (1DP). Overall, we have:

$$34.3451 \text{ (4DP)} + 34.5 \text{ (1DP)} = 68.8 \text{ (1DP)}$$

❖ **Rule 2 ($\times \div$)** *For multiplications and divisions, the number of significant figures of the result should be the same as the least number of significant figures involved.* For example, if you carry the following multiplication:

$$4500 \times 342 = 1500000 \text{ ($\times \div$ less SFs)}$$

the number 4500 (2SF) has two significant figures, whereas the number 342 (3SF) has three significant figures. If we multiply both numbers the results should contain just two significant figures. The result of multiplying 4500×342 is 1539000 (4SF), however, this number needs to be rounded into two significant figures into 1500000 (2SF). Overall we have:

$$4500 \text{ (2SF)} \times 342 \text{ (3SF)} = 1500000 \text{ (2SF)}$$

Sometimes we will have to add significant zeros in order to present the final result of a calculation with the correct number of digits. For example:

$$8.00 \text{ (3SF)} \div 2.00 \text{ (3SF)} = 4 \text{ (shows in calculator)} = 4.00 \text{ (3SF)}$$

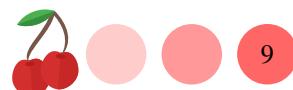
Sample Problem 4

Do the following calculation with the correct number of figures.

$$\frac{88.5 - 87.57}{345.13 \times 100}$$

SOLUTION

We will analyze each number indicating the number of SF and Digits (DP): 88.5(3SF, 1DP), 87.57(4SF, 2DP), 345.13(6SF, 2DP) and 100(1SF, 0DP). The



result of doing the addition needs to be rounded to one single decimal place: $88.5 - 87.57 = 0.93 \simeq 0.9$. After that we have only multiplications and divisions and hence we will now focus on the number of SFs:

$$\frac{0.9 \text{ (1SF)}}{345.13 \text{ (5SF)} \times 100 \text{ (1SF)}}$$

The result of this operation needs to be rounded to one SF:

$$\frac{0.9}{345.13 \times 100} = 2.6077 \times 10^{-5} \simeq 3 \times 10^{-5} \text{ (1SF)}$$

❖ STUDY CHECK

Do the following calculation with the correct number of figures: $(24.56 + 2.433) \times 0.013$

Rounding The following rules indicate how to round numbers:

❖ **Rule 1** If the digit to be removed is less than 5 then the preceding digit stays the same. For example, 1.123 rounds to 1.12.

❖ **Rule 2** If the digit to be removed is more or equal to 5 then the preceding digit is increased by one. For example, 1.126 rounds to 1.13

❖ **Rule 3** When rounding to a specific number of significant figures we need to look only to the first number to the right of the last significant figure. For example, 1.126 rounds to two SF as 1.1

Now, let us analyze a few use cases. Imagine we need to round the number 1234cm to two SF. The results would be 1200cm. Similarly, imagine we need to round the number 0.01264cm to two SF. The results would be 0.013cm.

Table 1.2 Different prefixes

Prefix	Symbol	Meaning	Value
exa	E	1000000000000000000	1×10^{18}
peta	P	1000000000000000000	1×10^{15}
tera	T	1000000000000	1×10^{12}
giga	G	1000000000	1×10^9
mega	M	1000000	1×10^6
kilo	k	1000	1×10^3
hecto	h	100	1×10^2
deca	da	10	1×10^1
–	–	1	1×10^0
deci	d	0.1	1×10^{-1}
centi	c	0.01	1×10^{-2}
milli	m	0.001	1×10^{-3}
micro	μ	0.00001	1×10^{-6}
nano	n	0.000000001	1×10^{-9}
pico	p	0.000000000001	1×10^{-12}
femto	f	0.000000000000001	1×10^{-15}
atto	a	0.000000000000000001	1×10^{-18}

1.4 Prefixes & Conversion Factors



Let's consider the following measurements: 1 km, 2 cm and 3 m that can be read as one kilometer, two centimeters, and three meters. The word **kilo** (**k**) and **centi** (**c**) are called **prefixed** whereas **meter** (**m**) is a simple unit. Table 1.2 lists some of the metric prefixes, their symbols, and their decimal values. A kilometer is larger than a meter, whereas a centimeter is smaller than a meter. Prefixes such as **kilo** or **centi** are attached to units to make numbers more manageable. For example, the radius of the earth is 6356 km, and this number is easier to handle than 6356000m. At the same time, we can attach any prefix to different units. Hence, we can talk about a centimeter (**cm**) but also about a centisecond (**cs**) or centiliter (**cL**). All these units have the same prefix.

How to identify prefixes? Look for example at the measurement 2 cm. **Centi** (**c**) is the prefix and means 1×10^{-2} and **meter** (**m**) is the unit that refers to length. Another example, is 7 kg read as seven kilograms. **Kilo** (**k**) is the prefix and means 1×10^3 , whereas **gram** (**g**) is the unit that refers to mass. The prefix refers to the first letter whereas the unit refers to the last letter.

A unit with a prefix can be bigger or smaller than the plain unit—this is the unit without a prefix—, depending on the prefix. The following prefixes reduce the unit: deci, centi, milli, micro, nano, pico, and femto. For example, a fs (femtosecond) is smaller than a s (second). Differently, the following prefixes increase the unit: Tera, Giga, Mega. For example, a Tb (terabyte) is larger than a b (byte). A byte is a unit used in computer science.

How to write unit equalities and conversion factors Unit equalities are simple expressions that relate a unit with a prefix. For example, one centimeter (**cm**) is $1 \times 10^{-2}m$. Hence we can write this as unit equality:

$$1\text{cm} = 1 \times 10^{-2}\text{m} \quad \text{unit equality}$$

Let's compare **cm** and **m**. The first, **cm**, is a unit with a prefix, whereas **m** is simply a unit of length without a prefix. To know how many **m** are there in a **cm** we need to write down a conversion factor. Think about prefixes as synonymous with a number. In this way, centi stands for 1×10^{-2} , so

$$\frac{1\text{cm}}{1 \times 10^{-2}\text{m}} \quad \text{or} \quad \frac{1 \times 10^{-2}\text{m}}{1\text{cm}} \quad \text{conversion factor}$$

The relationship above is also called a *unit factor* as both ratios are equal to one.

Sample Problem 5

Complete each of the following equalities and conversion factors:

(a) $1\text{dm} = \underline{\hspace{2cm}}\text{m}$ (c) $\frac{1\text{nm}}{\underline{\hspace{2cm}}\text{m}}$

(b) $1\text{km} = \underline{\hspace{2cm}}\text{m}$ (d) $\frac{\underline{\hspace{2cm}}\text{m}}{1\text{cm}}$

SOLUTION

(a) $1\text{dm} = 1 \times 10^{-1}\text{m}$; (b) $1\text{km} = 1 \times 10^3\text{m}$; (c) $\frac{1\text{nm}}{1 \times 10^{-9}\text{m}}$; (d) $\frac{1 \times 10^{-2}\text{m}}{1\text{cm}}$;

◆ STUDY CHECK

Second is a unit of time. Complete each of the following equalities and conversion factors involving seconds:

(a) $1\text{cs} = \underline{\hspace{2cm}}\text{s}$ (b) $\frac{\underline{\hspace{2cm}}\text{s}}{1\text{Ts}}$ (c) $\frac{\underline{\hspace{2cm}}\text{s}}{1\text{Ms}}$



1.5 Using Conversion Factors

Unit equalities in the form of conversion factors are used to convert one unit into another. Sometimes one wants to get rid of a prefix, such as when we transform centimeter (cm) into meter (m). Sometimes, one wants to convert a prefix into another prefix. An example would be converting centimeters (cm) to millimeters (mm). Let's work on some examples.

Removing or adding prefixes Imagine that you need to remove a prefix from a unit, and convert 3 km (we will call this one the original unit) into meters (this is the final unit). First, you would need the conversion factor corresponding to the prefix (centi) from Table 1.2. Then you need to arrange the conversion factor by placing the prefix at the bottom of the fraction. This will cancel out the prefix in the original unit and the bottom part of the conversion factor, hence leaving the final unit on top of the conversion factor. The arrangement would be:

$$3\text{km} \times \frac{1 \times 10^3 \text{m}}{1\text{km}} = 3000\text{m}$$

Imagine now that you need to add a prefix into a unit, and convert 4000 m in km. The same would apply for this case, but now you will have to arrange the conversion factor so that the prefix is on the top:

$$4000\text{m} \times \frac{1 \text{ km}}{1 \times 10^3 \text{m}} = 4\text{km}$$

Sample Problem 6

The length of a textbook page is 20cm. Convert 20cm to meters, expressing the result in scientific notation.

SOLUTION

In order to convert 20cm into meters, we need to remove the prefix (centi) leaving the unit (meter) without any prefix. We will use the conversion factor that relates m to cm: $\frac{1 \times 10^{-2} \text{m}}{1\text{cm}}$ or $\frac{1\text{cm}}{1 \times 10^{-2} \text{m}}$. We will arrange the conversion factor so that cm cancels giving m and hence we will use $\frac{1 \times 10^{-2} \text{m}}{1\text{cm}}$:

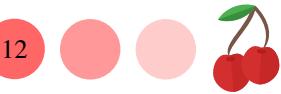
$$20\text{cm} \times \frac{1 \times 10^{-2} \text{m}}{1\text{cm}} = 2 \times 10^{-1}\text{m}$$

The original units and on the bottom of the conversion factor cancel and we get meters, the final unit.

❖ STUDY CHECK

Convert 100m to km, expressing the result in scientific notation.

Switching prefixes To switch a prefix into another prefix, such as transforming 30 millimeters (30 mm) into centimeters (cm), you will need two different conversion factors: the first conversion factor will remove the original unit (mm) introducing an intermediate unit, meters (m), whereas the second conversion factor will remove the intermediate meter and introduce the final unit (cm). You will get the conversion factors from Table 1.2. You will arrange the first conversion factor so that the original unit cancels out with the bottom of the first conversion factor, giving you an intermediate



unit. You will arrange the second conversion factor so that the intermediate unit cancels out with the bottom of the second conversion factor giving the final unit. For this example:

$$30\text{m}\cancel{\text{m}} \times \frac{1 \times 10^{-3}\text{m}}{1\text{m}\cancel{\text{m}}} \times \frac{1\text{cm}}{1 \times 10^{-2}\text{m}} = 3\text{cm}$$

Sample Problem 7

The length of a textbook page is 20cm. How many mm correspond this length, expressing the result in scientific notation.

SOLUTION

We want to convert 20 cm into mm, that is, we are switching prefixed. In order to do this, you need two conversion factors: $\frac{1 \times 10^{-2}\text{m}}{1\text{cm}}$ and $\frac{1\text{mm}}{1\text{mm}}$. You will have to arrange the number (20cm) and the two conversion factors in the following form:

$$20\text{cm} \times \frac{1 \times 10^{-2}\text{m}}{1\text{cm}} \times \frac{1\text{mm}}{1 \times 10^{-3}\text{m}} = 2 \times 10^2\text{mm}$$

◆ STUDY CHECK

Convert 100mm to km, expressing the result in scientific notation.

1.6 Units of volume and area

How big is your apartment? You might be living in a 750ft^2 loft in Brooklyn or a larger house Upstate. Often times we encounter cubic or square units such as cubic centimeters (cm^3) or square feet (ft^2). The equivalencies for cubic or square units should take into account the unit power (power of two or power of three). If $1\text{cm} = 1 \times 10^{-2}\text{m}$, for square units the relation should be squared and $1\text{cm}^2 = 1 \times (10^{-2})^2\text{m}^2 = 1 \times 10^{-4}\text{m}^2$. Another example, for the case of mm and mm^3 :

$$\boxed{\frac{1\text{mm}}{1 \times 10^{-3}\text{m}} \quad \text{and} \quad \frac{1\text{mm}^3}{1 \times 10^{-9}\text{m}^3}}$$

Let us work on an example in which we want to convert 30m^2 into m^2 :

$$30\text{m}\cancel{\text{m}} \times \frac{1\text{cm}^2}{1 \times 10^{-4}\text{m}\cancel{\text{m}}} = 3 \times 10^5\text{cm}^2$$

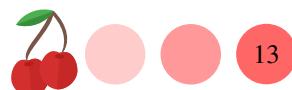
Sample Problem 8

How many m^2 is 20cm^2 , expressing the result in scientific notation.

SOLUTION

In order to convert 20cm^2 to square meters, we need to remove the centi prefix and that will give us the unit square meter without any prefix. We will use the conversion factor that relates m^2 to cm^2 : $\frac{1 \times 10^{-4}\text{m}^2}{1\text{cm}^2}$ or $\frac{1\text{cm}^2}{1 \times 10^{-4}\text{m}^2}$.

$$20\text{cm}\cancel{\text{m}} \times \frac{1 \times 10^{-4}\text{m}^2}{1\text{cm}\cancel{\text{m}}} = 2 \times 10^{-3}\text{m}^2$$



❖ STUDY CHECK

Convert $100m^3$ to dm^3 , expressing the result in scientific notation.

Table 1.3 Table containing some common unit equalities

Unit	Equality
Inches (in)-centimeters (cm)	$2.54^\dagger \text{ cm} = 1 \text{ in}$
miles (mi)-meters (m)	$1 \text{ mi} = 1609.34 \text{ m}$
minutes (min)-hours (h)	$60 \text{ min} = 1 \text{ h}$
minutes (min)-seconds (s)	$60 \text{ s} = 1 \text{ min}$
pound (lb)-grams (g)	$454 \text{ g} = 1 \text{ lb}$
cubic centimeter (cm^3)-mililiters (mL)	$1 \text{ mL} = 1 \text{ cm}^3$
Liter (L)-cubic decimeters (dm^3)	$1 \text{ L} = 1 \text{ dm}^3$
drops-mililiters* (mL)	$1 \text{ mL} = 15 \text{ drops}$

* There are several definitions of a drop

† the number is exact

Liters and milliliters Units such as L or mL are units of volume. As volume is a three-dimensional property, those units somehow have to be related to the units of length. One liter is the same as one dm^3 and one mL is the same as one cm^3 (See Figure 1.4). In the allied health field, the units mL are also written as cc as in cubic centiliters.

$$1\text{L} = 1\text{dm}^3 \text{ and } 1\text{mL} = 1\text{cm}^3(\text{cc})$$

Let us work on an example in which we want to convert $30cm^3$ into L:

$$30\text{cm}^3 \times \frac{1\text{mL}}{1\text{cm}^3} \times \frac{1 \times 10^{-3}\text{L}}{1\text{mL}} = 3 \times 10^{-2}\text{L}$$

Sample Problem 9

Convert $30 m^3$ into L, expressing the result in scientific notation.

SOLUTION

In order to convert m^3 into L we just need to remember that the L actually refers to dm^3 , therefore is connected to meter. We will first convert m^3 into dm^3 and then dm^3 into L.

$$30\text{m}^3 \times \frac{1\text{dm}^3}{1 \times 10^{-3}\text{m}^3} \times \frac{1\text{L}}{1\text{dm}^3} = 3 \times 10^4\text{L}$$

❖ STUDY CHECK

Convert 40L to cm^3 , expressing the result in scientific notation.

1.7 Using other equalities

How many hours are 300 minutes, or how many centimeters is 2 inches? Some of the units conversion is not based on a power of ten relationships and do not contain prefixes such as kilo or centi. Table 1.3 lists some of the common equalities that can be easily converted



into conversion factors. As an example, the unit equivalency between hours and minutes is $60\text{min} = 1\text{h}$ and the conversion factor would be $\frac{60\text{min}}{1\text{h}}$ or $\frac{1\text{h}}{60\text{min}}$.

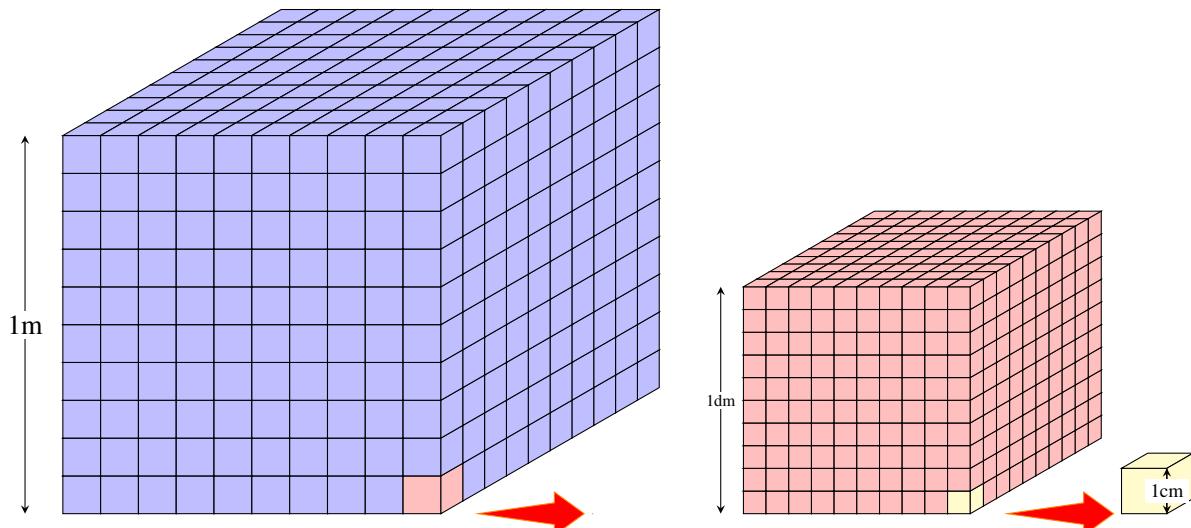


Figure 1.4 The left cube with a side of 1m has a volume of 1m^3 . The central cube with a side of 1dm has a volume of 1dm^3 , that is 1L. The right cube with a side of 1cm has a volume of 1cm^3 , that is 1mL.

Sample Problem 10

Convert 20 in to cm, expressing the result in scientific notation.

SOLUTION

We want to convert 20 inches into centimeters. The relationship between Inch and centimeter is given in Table 1.3. In order to do this, you need the conversion factor: $\frac{1\text{in}}{2.54\text{cm}}$ or $\frac{2.54\text{cm}}{1\text{in}}$. You will have to arrange the number (20 in) and the conversion factor in the following form:

$$20\cancel{\text{in}} \times \frac{2.54\text{cm}}{1\cancel{\text{in}}} = 5.080 \times 10^1\text{cm}$$

◆ STUDY CHECK

Convert 200mL to drops, expressing the result in scientific notation.

1.8 Measurements and uncertainty

Most chemistry experiments require the measurement of a property (mass, volume, temperature, color...), and the validity of those experiments will depend on the reliability of each measurement. The reliability of a measurement is usually considered in terms of its *accuracy* and its *precision*. At the same time, when experimenting oftentimes, one needs to repeat measurements. The results need to take into account the average measurement as well as the standard derivation of the series of results.

Uncertain and certain digits: how to report measured numbers

Consider the volume as measured in the glassware on the left side of Figure 1.5. Some would say the liquid meniscus occurs at 1.52mL. Mind we need to estimate the last number by interpolating between the 0.1mL marks. As the last digit of the number associated with the volume measurement is estimated, another person could measure



the volume as 1.53mL. The table below indicates the measurements of five different people.

Person	1	2	3	4
Volume(mL)	1.52	1.53	1.51	1.57

All measurements have in common the 1.5 part. The digit 5 is called a certain digit. The digit to the right of 5 is called the uncertain digit, as in a measurement it needs to be estimated. When reporting a measurement, we need to report up to the uncertain digit. These numbers on measurement are called *significant figures*. It is important to understand that all measured properties are subject to uncertainty. Uncertainty depends on one hand on the measuring device. The uncertainty on the left meniscus in Figure 1.5 is in the hundreds of the mL, whereas on the right meniscus occurs in the tenths of mL. Uncertainty also depends on the measurement process. As the uncertain digit needs to be reported in every measurement, the uncertainty on the last number on measurement is normally assumed to be ± 1 . For example, the right meniscus should be reported as $1.52 \pm 0.01\text{mL}$

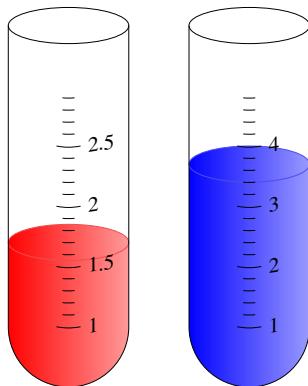


Figure 1.5 Two measuring devices. (Left side) The measuring device gives volumes to the hundredth place. (Right side) The measuring device gives volumes to the tenth place.

Precision and accuracy The terms precision and accuracy are two different terms often used to describe the reliability of measurement. Accuracy refers to the degree of agreement between the measured value and the true value, the real value of the property measured. Measurements that closely agree with the true value are accurate. Precision refers to the agreement between several measurements. Two measurements are accurate when they are close, independently of the true value of the property measured. Two different types of errors occur during a measurement. On one hand, random error refers to the fact that measured values can be above or below the true value. On the other hand, systematic error is an error that occurs each time in the same direction. Figure 1.6 displays accurate and inaccurate measurements as well as precise and imprecise measurements.

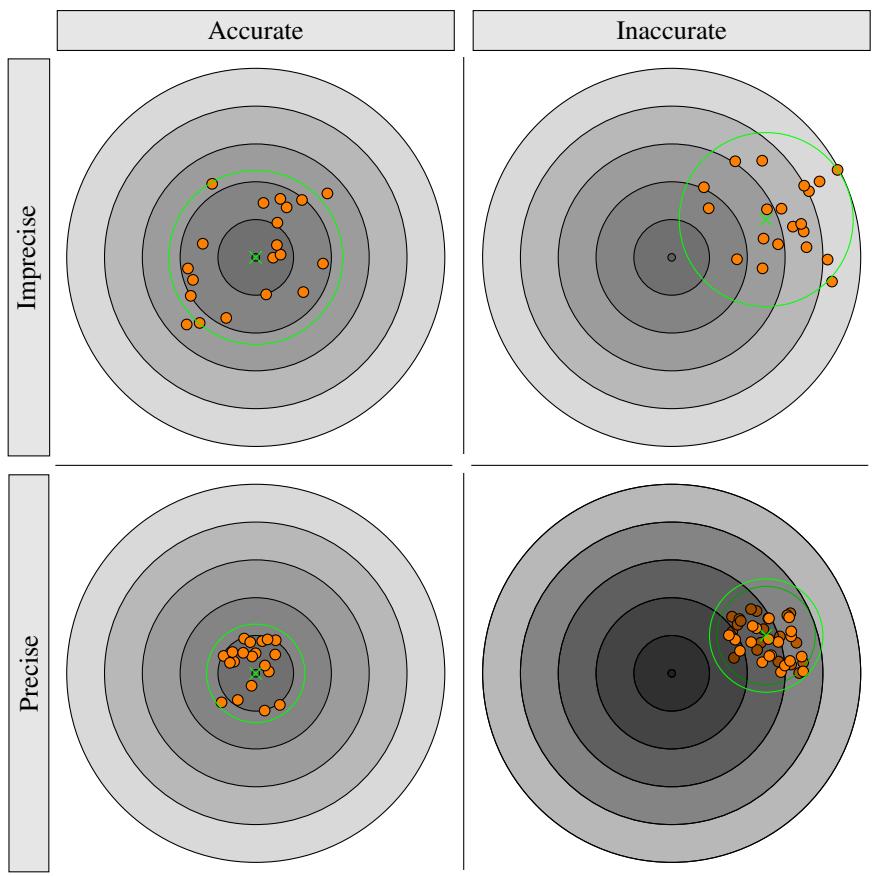


Figure 1.6 (Top Left) An accurate but imprecise measurement (Top Right) An inaccurate and imprecise measurement (Top Left) An accurate and precise measurement (Bottom Right) An inaccurate but precise measurement

Average and standard deviation The general approach to measuring a property such as the weight of a sample is to perform a number, n , of replicated measurements under similar conditions. Obtaining several measurements allows us to calculate the sample *average value*, \bar{x} , and the *standard deviation*, σ .

The sample average \bar{x} is calculated using the formula:

$$\bar{x} = \frac{1}{n} \sum_i^n x_i$$

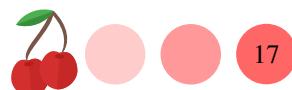
where $\sum_i^n x_i$ represents the sum of all measurements, x . The average value informs about the accuracy of the measurement. When the average is close to the true value the measurement is said to be accurate. The sample standard deviation σ provides estimates of the population values and it is calculated using the formula:

$$\sigma = \sqrt{\frac{1}{n-1} \sum_i^n (x_i - \bar{x})^2}$$

The final value for measurement should be written as:

$$x = \bar{x} \pm \sigma$$

notice that the standard deviation should have the same number of decimals as the average value. The standard deviation informs about the precision or dispersion of



the measurement. Very small standard deviations correspond to precise measurements. The following example demonstrates the calculation of the average and the standard deviation of a series of measurements.

Sample Problem 11

We measured the mass of the same sample several times obtaining the following values: 108.6 g, 104.2 g, 96.1 g, 99.6 g, and 102.2 g. Answer the following questions: (a) Compute the average, \bar{x} . (b) Compute the standard deviation of the measurement, σ . (c) Report the measured mass in the form $\bar{x} \pm \sigma$.

SOLUTION

(a) The average mass is given by:

$$\bar{m} = \frac{1}{5}(108.6\text{ g} + 104.2\text{ g} + 96.1\text{ g} + 99.6\text{ g} + 102.2\text{ g}) = 102.1\text{ g}.$$

(b) The standard deviation is given by:

$$\begin{aligned}\sigma = \sqrt{\frac{1}{4} \left((108.6\text{ g} - 102.1\text{ g})^2 + (104.2\text{ g} - 102.1\text{ g})^2 + (96.1\text{ g} - 102.1\text{ g})^2 \right.} \\ \left. + (99.6\text{ g} - 102.1\text{ g})^2 + (102.2\text{ g} - 102.1\text{ g})^2 \right)} = 4.7\text{ g}.\end{aligned}$$

(c) The measured mass is given by: $102.1 \pm 4.7\text{ g}$

◆ STUDY CHECK

We measured the volume of the same sample several times obtaining the following values: 10.12 mL, 10.12 mL, 10.13 mL, 10.14 mL, and 10.15 mL. Answer the following questions: (a) Compute the average, \bar{x} . (b) Compute the standard deviation of the measurement, σ . (c) Report the measured volume in the form $\bar{x} \pm \sigma$. (d) Given that the true volume is 10.50 mL, describe the accuracy and precision of the measurement

1.9 Matter

Matter—the material of the universe—represents anything with mass that occupies space. It has different levels of organization and complexity. We can classify matter in terms of composition. Some substances are made of a single component whereas others contain multiple components. At the same time, some substances are made of many components while they appear to be made of a single component. Figure 1.7 displays the classification of matter in terms of mixture nature and composition.

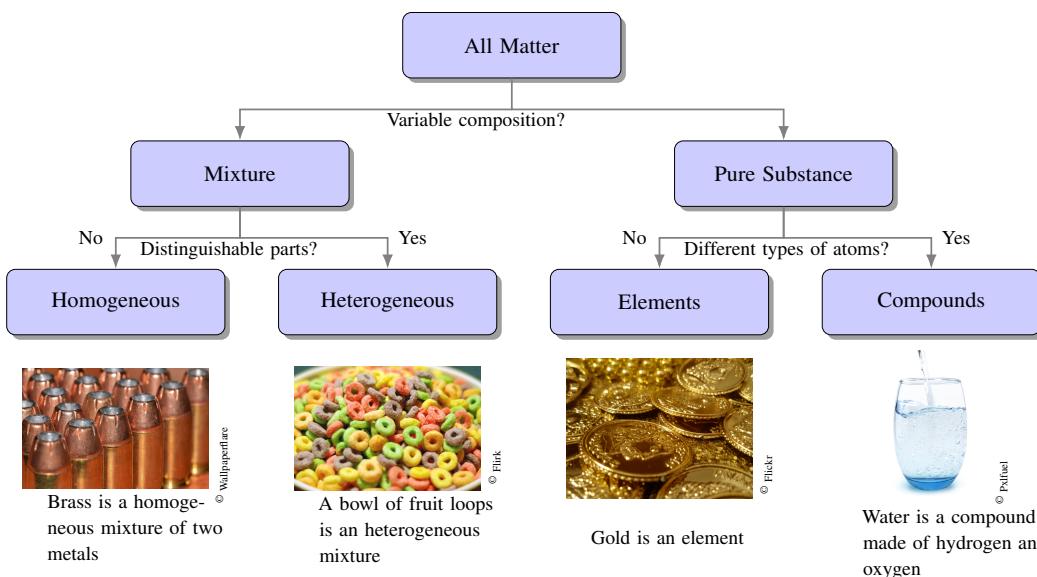


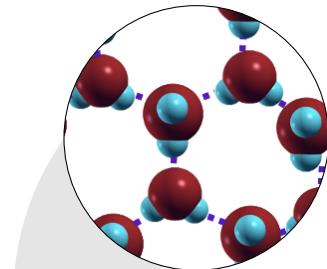
Figure 1.7 Classification of the matter

Solids, liquids & gases *Solid* has a well-defined shape and volume. Think about an ice cube, for example, that is made of water in the form of ice. In an ice cube, attractive forces keep the shape of the cube constant. The water molecules in the ice are arranged in rigid patterns and they can only vibrate in the solid. A *liquid*, on the other hand, has a well-defined volume. However, liquids do not have a constant shape, as their shape will depend on the shape of the container. Think about water which is a liquid. You can find many different bottle shapes. In all of them, the molecules of water will arrange to occupy the shape of the container. The volume of the liquid—the amount of space the liquid occupies—will be constant but not the shape. In a liquid, the particles move randomly but are still attached. A *gas* does not have a well-defined shape or volume. In a gas, the particles are randomly distributed and barely interact with each other, as they move at high speeds, taking the shape and volume of their container. Figure 1.8 displays the microscopic structure of the three different states of matter of water. The process of boiling and freezing represent *physical changes* and during physical changes, these substances involved do not change their composition. When water boils, both steam and water are made of the same component, H_2O . When a substance undergoes a *chemical process*, it will change its composition. For example, when burning a piece of paper, paper made of carbon, hydrogen, and oxygen becomes ash made mostly of carbon. As such, during a chemical process, a substance (e.g. paper) becomes a new substance (e.g. carbon).

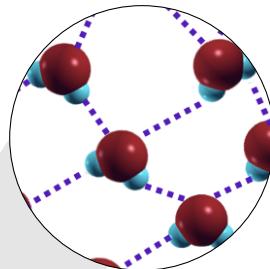
Pure Substances and mixtures On one hand, *pure substances* have definite composition, being only made of a single component. For example, water and gold are pure substances. However, there are two different types of pure substances: elements and compounds. *Elements* is composed of only one type of atom. Examples are silver, iron, and aluminum. They all contain one type of substance, and for example, iron is only made of iron atoms. *Compounds* are combinations of different elements. For example, water, H_2O is a compound made of a combination of hydrogen and oxygen atoms. On the other hand, *mixtures* are physical combinations of different pure substances. Mixtures have variable compositions. For example, the air is a mixture of oxygen and nitrogen. Wood, soda pop, or soil are all mixtures. Mixtures can be homogeneous or heterogeneous. In a *homogeneous mixture*—also known as solutions—the composition is uniform throughout the sample. An example of a homogeneous

mixture is salty water, a solution of salt and water. *Heterogeneous mixtures* are mixtures in which the components are not uniformly distributed throughout the sample. An example would be a chocolate chip cookie in which you can differentiate the dough and the chocolate.

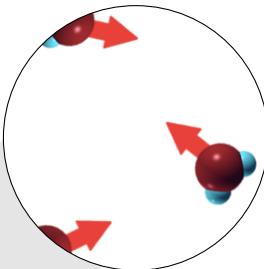
▼The molecular hexagonal structure of ice, solid water.



▼The molecular structure of liquid water.



▼The molecular structure of steam, gaseous water.


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Figure 1.8 Three different states of matter, solid, liquid, and gas. Solid molecules are locked into fixed positions, while liquid molecules are together but still can move. Gas molecules are apart and move freely.

Sample Problem 12

Classify as element, compound, homogeneous mixture, heterogeneous mixture:

- (a) An iron nail (b) Milk (c) Sugar (d) miso soup

SOLUTION

(a) An iron nail is an element as it is only made of iron, a single material; (b) Milk is a homogeneous mixture as it is made of water, fat, protein even though you only see a single substance; (c) Sugar is a compound made of carbon and other constituents; (d) miso soup is a mixture of water, fat and other chemicals and therefore is a mixture. As you can differentiate its constituents we call this heterogeneous mixture.

◆ STUDY CHECK

Classify as element, compound, homogeneous mixture, heterogeneous mixture:

- (a) muscle milk (b) water (c) a gold ring (d) rice & beans

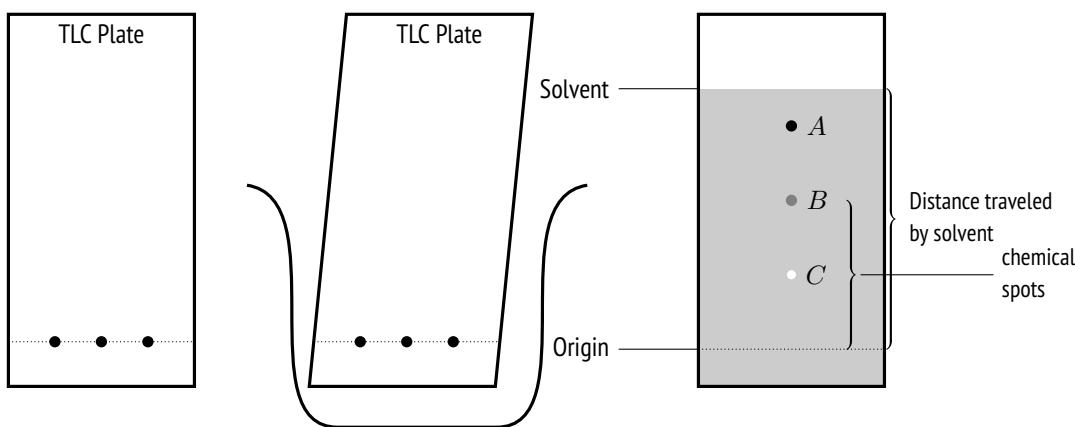
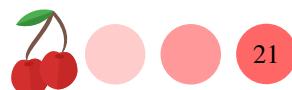


Figure 1.9 TLC set up. (Left) Solid phase with spots (Center) Solid phase inside a beaker containing the liquid phase (Right) Solid phase with separated mixture components.

Separation Techniques Chemists and scientists often need to separate the components of a mixture. There are many analytical techniques used to separate and identify the components of a mixture. These techniques exploit the differences in the chemical or physical properties of the components of the mixture to separate the different elements. The techniques used to separate mixtures are called *separation techniques*. Distillation is an important separation technique used to separate compounds with different volatility—different tendencies to generate vapor. For example, a mixture containing water and gasoline can be distilled as the components of the mixture largely differ in their volatility. The distillation setup consists of a distilling flask containing the mixture to be distilled, a condenser, and a receiving flask. When the mixture is heated the most volatile component will separate first and with the help of the condenser—a cooled tube—will cool down into liquid and deposit on the receiving flask. It is important to understand that only mixtures of liquids or mixtures of solids and liquids can be distilled. Another important separation technique is *filtration*. This technique is used to separate mixtures of solids and liquids. The mixture to be filtered is poured into a mesh—for example a filter—that retains the solid and lets the liquid pass. *Chromatography* is another separation technique. Indeed, the name represents a series of methods that uses two different phases, a mobile phase, and a stationary phase, to separate the components of a mixture. The principle behind this technique is the differences in affinity of the mixture components towards the mobile and stationary phases. The stationary phase is a solid whereas the mobile phase can either be a liquid (paper chromatography) or a gas (gas chromatography). Mixture components with a high affinity for the mobile phase will move faster through the chromatographic system. *Thin layer chromatography* (TLC) relies on capillarity, which is the tendency of liquid substances to rise on the surface of a material (Figure 1.9). In this technique, a drop of a liquid solution containing different substances (the sample) is deposited on a rectangular piece of filter paper, close to the bottom edge. This paper is called the stationary phase. The bottom end of the paper is immersed in a liquid called the mobile phase, to a point that is just below the spot where the sample was placed. Due to capillarity, the mobile phase will move up along the stationary phase. When the mobile phase reaches the sample, the different components of the mixture will begin to migrate, carried away by the mobile phase. The chemical compounds forming the sample will move with the mobile phase, but as different chemicals have different tendencies to stick to the mobile



phase, they will cover different distances in the stationary phase. The different heights achieved by the different substances would allow you to identify those chemicals. A component of the mixture with a high affinity to the mobile phase will migrate more than a component with a higher affinity to the stationary phase. The distance traveled by a component referred to as the distance traveled by the mobile phase is a measure of the affinity between the chemical and the mobile phase. The *retention factor* R_f of a given chemical is defined as:

$$R_f = \frac{\text{distance traveled by the chemical}}{\text{total distance traveled by mobile phase}}$$

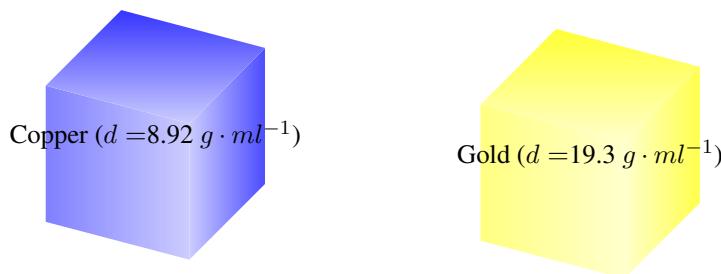
The R_f value of a substance is characteristic of that substance. When dealing with mixtures one has to calculate the R_f for each pure component separately to then compare the retention factors with the ones obtained in the mixture.

1.10 Density

Density refers to the mass of a substance with respect to its volume. This is an unique property for each substance. Table 1.4 reports the density of numerous substances. Indeed, density is often used as an identification tag. The formula for density is

$$\text{Density} = \frac{\text{Mass of substance}}{\text{Volume of substance}} \quad (1.1)$$

For example, the density for copper is $8.92 \text{ g} \cdot \text{ml}^{-1}$ and for gold is $19.3 \text{ g} \cdot \text{ml}^{-1}$. By measuring density only, you would be able to differentiate copper than gold. The larger density the more compact is an object and that means the more mass per volume it has. At the same time, for the same volume, the larger density the larger the mass of the metal.



Density and mixing A small piece of ice will float on the water. The reason for that is density: the density of ice (0.9g/mL) is smaller than the density of water (1.0g/mL) and hence ice will stay on top of the water. Objects with a density larger than 1 g/mL will sink whereas objects with a density smaller than this value will float. Figure 1.10 showcases how objects with density larger than water will sink whereas objects with a smaller density will float. If you add a drop of vegetable oil to a glass of water, the drop will float. This is because the density of oil is smaller than 1g/mL .

**Table 1.4 Density of some common substances at 273.15 K and 100 kPa**

Substance	Density (g/mL)	Physical State
Helium	0.2	gas
Hydrogen	0.1	gas
Water	1.0	Liquid
Cooking oil	0.9	Liquid
Mercury	13.5	Liquid
Tetrachloroethene	1.6	Liquid
Gold	19.3	solid
Plastics	1.2	solid
Ice	0.916*	solid

*Ice is given at T < 273.15 K

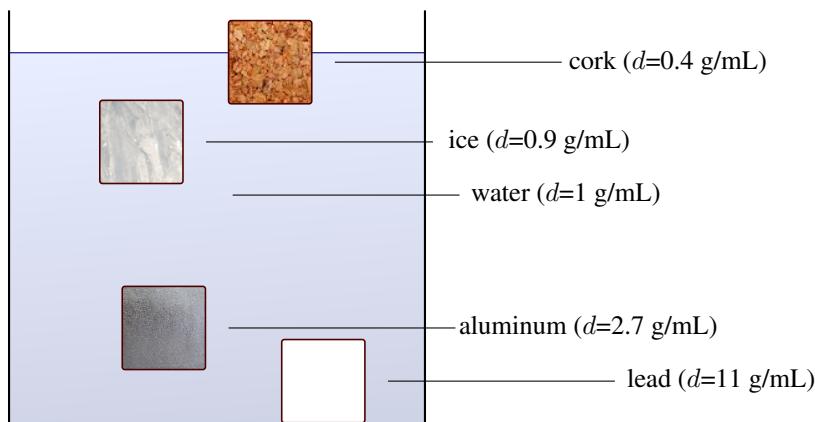


Figure 1.10 Objects with a larger density than water will sink whereas objects with a smaller density will float.

Sample Problem 13

In the figure, we mixed three liquids of density: A (0.5 g/mL), B(2 g/mL) and C(1 g/mL). Identify each liquid.

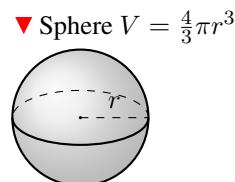
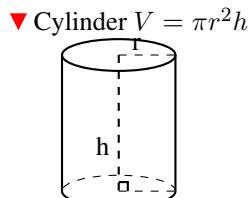
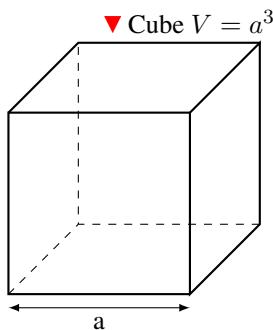
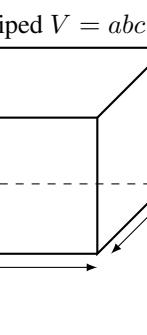
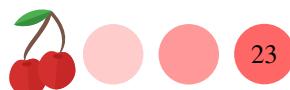


SOLUTION

The heavier the liquid, that is the larger density, the lower the liquid will arrange in the mixture. From top to bottom we have A, C and B.

◆ STUDY CHECK

Indicate the order that the following invisible liquids will appear in a cylinder when mixed: (a) benzene(0.87 g/mL) and (b) water(1 g/mL)



Volume of some objects

Density and the volume of objects Density depends on volume and in particular the larger volume the smaller density. Figure 1.11 displays the formulas to calculate the volume for some common objects, like a sphere or a cube. For example, the radius of a sphere with density d and mass m corresponds to $\sqrt[3]{3m/4d \cdot \pi}$, and the side of a cube with density d and mass m corresponds to $\sqrt[3]{m/d}$. The density of liquids results from measuring the mass of a given volume of the liquid. Differently, density is harder to obtain for solids. For metals, we can calculate density by the immersion method: when a metal is immersed in water, the water rises. This increase in volume corresponds to the volume of the solid. This way, density results from the direct measurement of mass and the measurement of volume by displacement.

The following example demonstrates density calculation with the immersion method.

Sample Problem 14

After adding a 30g object into a cylinder filled of water, the level of water rises from 60mL to 90mL. Calculate the density of the object.

SOLUTION

Density is mass over volume. The mass of the object is 30g and its volume is (90-60)mL that is 30mL. Hence: $d = 30g/30mL = 1g/mL$.

◆ STUDY CHECK

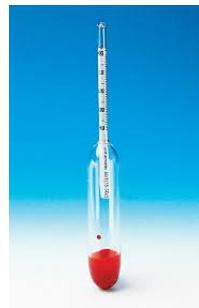
A lead weight used in the belt of a scuba diver has a mass of 226 g. When the weight is placed in a graduated cylinder containing 200.0 mL of water, the water level rises to 220.0 mL. What is the density of the lead weight (g/mL)?

Specific gravity The specific gravity (ρ) of a substance is the ratio between its density and the density of a reference, normally water. It is simply calculated by dividing the density of the substance and the density of water (1g/mL at room temperature).

$$\rho = \frac{\text{density of substance}}{\text{density of water}} \quad (1.2)$$

A substance with a specific gravity of 1 has a density of 1g/mL. This is a unitless property that can be measured with an instrument called a hydrometer. For example, the specific density of the urine in the body is used to identify diabetes or kidney malfunctioning.

▼A hydrometer



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▼Dipstick used to measure specific gravity



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CHAPTER 1

MATH SKILLS

1.1 Solve for x in the following algebraic equations:
 (a) $\frac{3x+1}{2} = 2$ (b) $\frac{2x-1}{3} = 2$ (c) $\frac{2}{3} = \frac{1}{3x}$

1.2 Solve for x in the following algebraic equations:
 (a) $3x + 1 = 5$ (b) $2x - 1 = 5$ (c) $\frac{3}{2} = \frac{1}{2x}$

1.3 Compute the following calculations involving scientific notation: (a) $\frac{6.5 \times 10^3}{3 \times 10^2}$ (b) $\frac{6.1 \times 10^{-3}}{3 \times 10^4}$ (c) $\frac{1.3 \times 10^{-3}}{2.5 \times 10^{-2}}$

1.4 Compute the following calculations involving scientific notation: (a) $\frac{2.4 \times 10^{-3}}{(5)(4.6 \times 10^{-6})}$ (b) $\frac{1}{(3)(4 \times 10^{-1})}$
 (c) $\frac{1}{(4)(1 \times 10^{-4})}$

UNITS OF MEASUREMENTS AND SYSTEMS OF UNITS

1.5 Indicate the magnitude measured in the following measurements: (a) 2 L (b) 5 cm

1.6 Indicate the magnitude measured in the following measurements: (a) 100 Kg (b) 10h

1.7 Answer the following questions: (a) Indicate the metric base unit for mass (b) Indicate the metric base unit for time (c) Indicate metric base unit for volume

1.8 Answer the following questions: (a) Indicate basic unit of mass in the SI (b) What magnitude measures the amount of space occupied by a substance

SIGNIFICANT FIGURES

1.9 Indicate if the following statements represent measured or exact numbers: (a) The number of apples in a bag (b) The weight of an apple (c) The number of cm in a inch

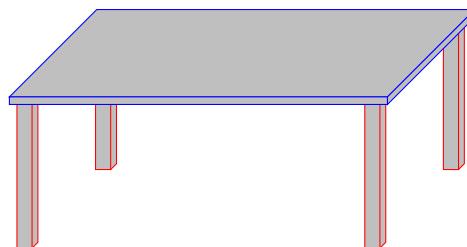
1.10 Indicate if the following statements represent measured or exact numbers: (a) The number of students in a classroom (b) The height of a student

1.11 Identify the following numbers as measured or exact: (a) The number of students enrolled in a class is 25

(b) The temperature of a sample is $25^\circ C$ (c) The mass of an object is 10 Kg (d) 1000grams is 1Kg

1.12 Identify the following numbers as measured or exact: (a) The length of an object is 4 cm (b) A chair has four legs (c) The density of a solution is 0.6 g/mL (d) One meter equals 100 cm

1.13 Identify the following numbers as measured or exact given the image below:



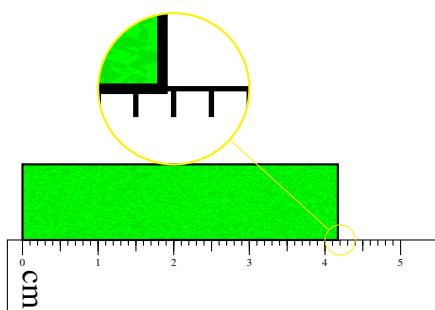
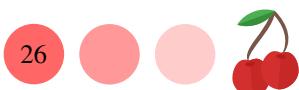
(a) The height of the table (b) The number of table legs
 (c) The width of the table (d) The number of tables in the image

1.14 Identify the following numbers as measured or exact given the image below:

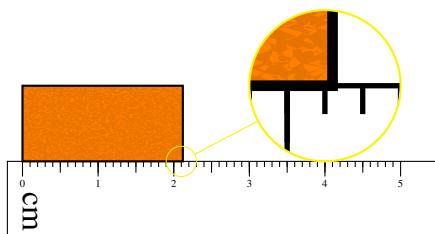


(a) The weight of the tiger (b) The number of ears of the tiger (c) The height of the tiger (d) The number of whiskers

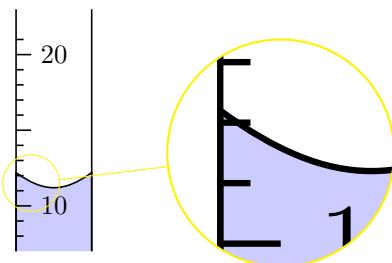
1.15 Give the following measurement with the correct number of digits, while indicating the number of significant figures of the measurement and the estimated digit.



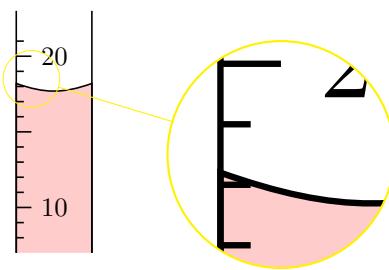
- 1.16** Give the following measurement with the correct number of digits, while indicating the number of significant figures of the measurement and the estimated digit.



- 1.17** Give the following measurement in mL with the correct number of digits, while indicating the number of significant figures of the measurement and the estimated digit.



- 1.18** Give the following measurement in mL with the correct number of digits, while indicating the number of significant figures of the measurement and the estimated digit.



- 1.19** Indicate the number of SFs. (a) 0.0032 m (b) 5100 m (c) 0.510 m (d) 0.0051 m (e) 500 m (f) 45.030

- 1.20** Which of the following measurements contains the designated CORRECT number of significant figures? (a) 0.05600 cm (5 SF) (b) 0.03040 cm (3 SF) (c) 456 000 cm (3 SF) (d) 1.304 cm (2 SF) (e) 3.12050 cm (4 SF)

- 1.21** Carry the following calculations with the correct number of digits or significant figures:

$$\begin{array}{ll} \text{(a)} & 0.2301 + 0.123 \\ \text{(b)} & 0.2301 - 1.12 \end{array} \quad \begin{array}{ll} \text{(c)} & 88.1 - 87.57 \\ \text{(d)} & 24.56 + 2.4 \end{array}$$

- 1.22** Carry the following calculations with the correct number of digits or significant figures:

$$\begin{array}{ll} \text{(a)} & 523 \times 5000 \\ \text{(b)} & 5 / 0.123 \end{array} \quad \begin{array}{ll} \text{(c)} & 27.0 \times 0.01 \\ \text{(d)} & 345.13 / 100 \end{array}$$

- 1.23** Round the following numbers to 3SFs: (a) 12849m (b) 5111s (c) 2.4566×10^{-3} Kg (d) 0.051376cm (e) 573456mm (f) 0.0293845 μ m

- 1.24** Round the following numbers to 1SFs: (a) 12849m (b) 5111s (c) 2.4566×10^{-3} Kg (d) 0.051376cm (e) 573456mm (f) 0.0293845 μ m

PREFIXES & CONVERSION FACTORS

- 1.25** Fill the gap in the following unit equalities or conversion factors: $1Km =$ m

- 1.26** Fill the gap in the following unit equalities or conversion factors: $1cm =$ m

- 1.27** Fill the gap in the following unit equalities or conversion factors: $\frac{1nm}{\text{_____} m}$



1.28 Fill the gap in the following unit equalities or conversion factors: $\frac{1fs}{\text{[] s}} = \text{[]}$

1.29 Fill the gap in the following unit equalities or conversion factors:

$$\begin{array}{ll} 1Tm = \text{[] m} & 1qt = \text{[] mL} \\ 1dm = \text{[] m} & 1L = \text{[] dm}^3 \\ 1cg = \text{[] g} & 1lb = \text{[] g} \\ 1ms = \text{[] s} & 1in = \text{[] cm} \end{array}$$

1.30 Fill the gap in the following unit equalities or conversion factors:

$$\begin{array}{ll} (\text{a}) \frac{1\text{km}}{\text{[] m}} & (\text{d}) \frac{\text{[] L}}{10^{-3}\text{L}} \\ (\text{b}) \frac{1\text{cm}}{\text{[] m}} & (\text{e}) \frac{\text{[] L}}{10^{-2}\text{L}} \\ (\text{c}) \frac{1\text{ms}}{\text{[] s}} & (\text{f}) \frac{\text{[] g}}{10^{-1}\text{g}} \end{array}$$

USING CONVERSION FACTORS

1.31 Fill the gap in the following unit conversion:

$$70\text{cm} \times \frac{\text{[] m}}{1\text{cm}} = 0.7m$$

1.32 The following conversion factor is used to convert $100\mu\text{m}$ into m. Fill in the gaps:

$$100\mu\text{m} \times \frac{\text{[] m}}{1\mu\text{m}} = 1 \times 10^{-4}m$$

1.33 The following conversion factor is used to convert 40m into nm. Fill in the gaps:

$$40\text{m} \times \frac{1\text{nm}}{\text{[] m}} = 4 \times 10^{10}\text{nm}$$

1.34 The following conversion factor is used to convert 500m into μm . Fill in the gaps:

$$500\text{m} \times \frac{1\mu\text{m}}{\text{[] m}} = 5 \times 10^8\mu\text{m}$$

1.35 Complete the following unit conversion:

$$100Gm \times \frac{\text{[] m}}{Gm} = \text{[] m}$$

1.36 Complete the following unit conversion:

$$50km \times \frac{\text{[] m}}{km} = \text{[] m}$$

1.37 Complete the following unit conversion:

$$2\text{m} \times \frac{\text{[] cm}}{\text{[] m}} = \text{[] cm}$$

1.38 Complete the following unit conversion:

$$0.3\text{m} \times \frac{\text{[] mm}}{\text{[] m}} = \text{[] mm}$$

1.39 Complete the following unit conversion:

$$\begin{array}{l} (\text{a}) 0.5\mu\text{g} \times \frac{\text{[] g}}{\mu\text{g}} = \text{[] g} \\ (\text{b}) 125\text{L} \times \frac{\text{[] mL}}{\text{[] L}} = \text{[] mL} \end{array}$$

1.40 Complete the following unit conversion:

$$\begin{array}{l} (\text{a}) 100\text{nm} \times \frac{\text{[] m}}{\text{[] nm}} = \text{[] m} \\ (\text{b}) 10\text{dm} \times \frac{\text{[] m}}{\text{[] dm}} = \text{[] m} \end{array}$$

1.41 The following conversion factor is used to convert 30cm into km. Fill in the gaps:

$$30\text{cm} \times \frac{\text{[] m}}{1\text{cm}} \times \frac{1\text{km}}{\text{[] m}} = 3 \times 10^{-4}\text{km}$$

1.42 The following conversion factor is used to convert 50dm into cm. Fill in the gaps:

$$50\text{dm} \times \frac{\text{[] m}}{1\text{dm}} \times \frac{1\text{cm}}{\text{[] m}} = 500\text{cm}$$

1.43 Fill the gap in the following conversion factors:

$$20\text{cm} \times \frac{1 \times 10^{-2}\text{m}}{1\text{cm}} \times \frac{1\text{mm}}{1 \times 10^{-3}\text{m}} = \text{[] mm}$$

1.44 Fill the gap in the following conversion factors:

$$5\text{mm} \times \frac{1 \times 10^{-3}\text{m}}{1\text{mm}} \times \frac{1\text{nm}}{1 \times 10^{-9}\text{m}} = \text{[] nm}$$



1.45 Set up the conversion factor to convert 50cm into inches:

$$50\text{ cm} \times \frac{\text{_____}}{\text{_____}} = \text{_____ in}$$

1.46 Fill the gap in the following conversion factors:

$$20\text{ cm} \times \frac{\text{_____}}{\text{_____}} = 7.87\text{ in}$$

1.47 Compute the following power of ten calculations:

- | | |
|----------------|-------------------|
| (a) $(10^2)^2$ | (c) $(10^{-6})^2$ |
| (b) $(10^2)^3$ | (d) $(10^{-2})^2$ |

1.48 Compute the following power of ten calculations:

- | | |
|----------------|-------------------|
| (a) $(10^1)^3$ | (c) $(10^{-5})^2$ |
| (b) $(10^3)^4$ | (d) $(10^{-4})^5$ |

1.49 Set up the following conversion factor:

$$400\text{ cm}^2 \times \frac{\text{_____}}{\text{_____}} = \text{_____ m}^2$$

1.50 Set up the following conversion factor:

$$0.4\text{ pm}^3 \times \frac{\text{_____}}{\text{_____}} = \text{_____ m}^3$$

1.51 Fill the gap in the following unit equalities or conversion factors:

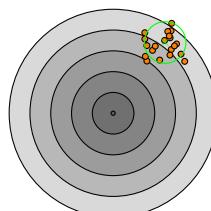
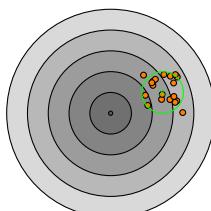
$$\begin{array}{ll} 1\text{ cm}^2 = \text{_____ m}^2 & 1\text{ cm}^3 = \text{_____ m}^3 \\ 1\text{ dm}^3 = \text{_____ m}^3 & 1\text{ dm}^2 = \text{_____ m}^2 \end{array}$$

1.52 Fill the gap in the following unit equalities or conversion factors:

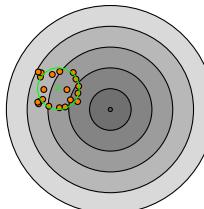
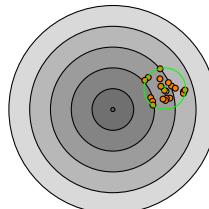
$$\begin{array}{ll} 1\text{ mm}^2 = \text{_____ m}^2 & 1\text{ }\mu\text{m}^2 = \text{_____ m}^2 \\ 1\text{ nm}^2 = \text{_____ m}^2 & 1\text{ km}^2 = \text{_____ m}^2 \end{array}$$

MEASUREMENTS AND UNCERTAINTY

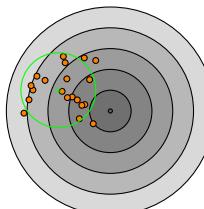
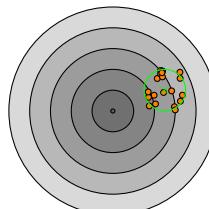
1.53 Compare the precision and accuracy of the following measurements:



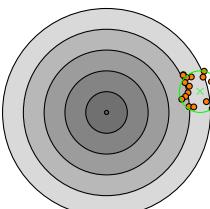
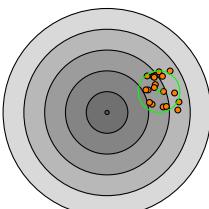
1.54 Compare the precision and accuracy of the following measurements:



1.55 Compare the precision and accuracy of the following measurements:



1.56 Compare the precision and accuracy of the following measurements:

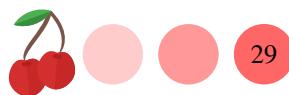


MATTER

1.57 Classify the following objects as an element, compound, and homogeneous mixture, a heterogeneous mixture or none of the others: (a) an energy drink (b) helium (a gas) (c) sulfur (a solid) (d) milk (e) milkshake (f) gelato (g) air (h) granite (i) uranium (a solid)

1.58 Classify the following objects as an element, compound, and homogeneous mixture, a heterogeneous mixture or none of the others: (a) a copper wire (b) a chocolate cookie (c) a chocolate-chip cookie (d) vinegar (e) ice (f) baking soda (g) aluminum foil (h) vitamin C

1.59 Which of the following is a property of a solid? (a) It takes the shape of the container. (b) It fills the volume of the container. (c) The particles move at a rapid rate. (d) The interactions between its particles are very weak. (e) The particles have fixed positions and are very close together.



1.60 Which of the following is a property of a liquid?
 (a) It takes the shape of the container. (b) it has no volume.
 (c) The particles move at a rapid rate. (d) The interactions between its particles are unexistent. (e) The particles have fixed positions and are very close together.

1.61 Which of the following is a property of a gas?
 (a) It has no shape. (b) It fills the volume of the container.
 (c) The particles move slowly. (d) The interactions between its particles are strong. (e) The particles have fixed positions and are very close together.

1.62 Which of the following is a property of a gas and a liquid? (a) It flows. (b) It takes the shape of the container.
 (c) It has no shape. (d) It fills the volume of the container.
 (e) The particles move slowly. (f) The interactions between its particles are strong. (g) The particles move at a rapid rate. (h) The interactions between its particles are unexistent. (i) The particles have fixed positions and are very close together.

DENSITY

1.63 Determine the density (g/mL) of a 0.01 L sample of a salt solution that has a mass of 50 g.

1.64 Determine the density (g/mL) of a 0.05 L sample of a salt solution that has a mass of 10 g.

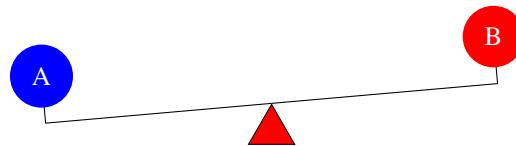
1.65 Which one of the following substances will float in gasoline, which has a density of 0.66 g/mL? Assume no mixing: (a) table salt (2.16 g/mL) (b) balsa wood (0.16 g/mL) (c) sugar (1.59 g/mL) (d) aluminum (2.70 g/mL)
 (e) mercury (13.6 g/mL)

1.66 You have a large water tank used as a cooler in a party and you have a bunch of cans: a coke can, a diet coke can, a water can and a schweppes can. You add all unopened cans on the tank. Describe the final vertical distribution of cans in the tank. Which can will stay on top and which will sink in more?

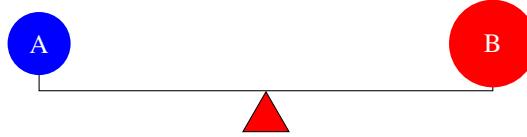
1.67 A nugget of gold with a mass of 521 g is added to 50.0 mL of water. The water level rises to a volume of 77.0 mL. What is the measured density of the gold?

1.68 A graduated cylinder contains 28.0 mL of water. What is the new water level after 35.6 g of silver metal is submerged in the water if the density of silver is 10g/mL?

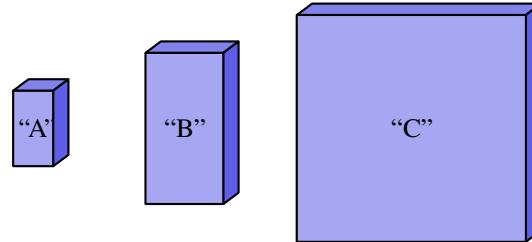
1.69 Which of the circles is more dense: A or B.



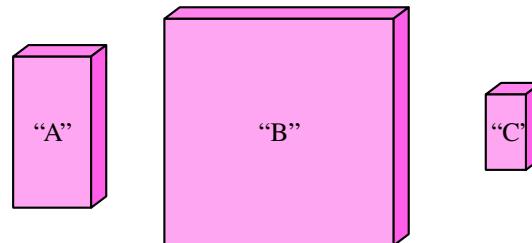
1.70 Which of the circles is more dense: A or B.



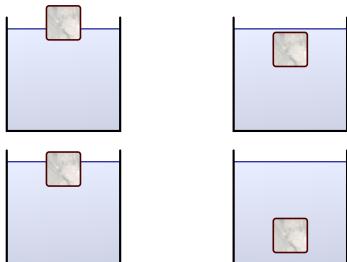
1.71 The objects below have all the same mass but represent different metals cobalt, gold, and palladium. Given that the density of cobalt is 8g/mL, whereas the density of gold is 19g/mL and the density of palladium is 12g/mL, identify each object as cobalt, gold, and palladium.



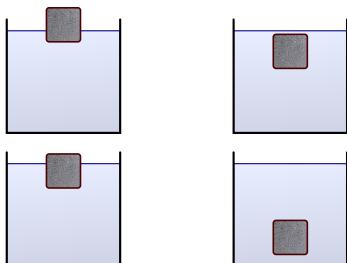
1.72 The objects below have all the same mass but represent different metals iron, nickel, and tungsten. Given that the density of iron is 7g/mL, whereas the density of nickel is 9g/mL and the density of tungsten is 20g/mL, identify each object as iron, nickel, or tungsten.



1.73 The diagrams below represent a solid immersed in a liquid, with some of the solids floating and others sinking. Match the diagrams with the description: (a) The density of the solid is 1.1 times the density of the liquid
 (b) The density of the solid is the same the density of the liquid (c) The density of the solid is 0.8 times the density of the liquid (d) The density of the solid is 0.5 times the density of the liquid



1.74 The diagrams below represent a solid immersed in a liquid of density 0.9g/mL, with some of the solids floating and others sinking. Match the diagrams with the description: (a) The density of the solid is 1.2g/mL (b) The density of the solid is 0.9g/mL (c) The density of the solid is 0.7g/mL (d) The density of the solid is 0.4g/mL



1.75 Answer the following questions involving specific gravity: (a) A sample has a density of 0.9g/mL. How much is its specific gravity? (b) A sample has a specific gravity of 1.20. How much is its density? (c) True or false: an orange juice sample should have a specific gravity larger than one.

1.76 Answer the following questions involving specific gravity: (a) True or false: an olive oil sample should have a specific gravity larger than one. (b) A sample has a mass of 5mg and a specific gravity of 0.87. Calculate its volume in mL.

1.77 Answer the following questions involving dosages: (a) An IV solution needs to be delivered at a rate of 120mL/h. How long it takes to deliver 200mL? (b) Infant Tylenol is given from a 160mg/5mL suspension based on the infant's weight. A 12lb infant requires 2.5mL. How many milligrams of Tylenol are contained in the dosage given?

1.78 Answer the following questions involving dosages:

(a) A patient requires 1g of medication given every three hours. The medication in stock was found in tablets of 200mg. How many tablets do you need in three days?

(b) A medication needs to be given based on the patient's body weight as 2mg/Kg. If a patient weighs 70Kg and the medication stock is 100mg/mL, how many mL are needed?

Ch. 2. The periodic table: atoms and Elements

MATTER is everywhere around you, from the water you drink to the air you inhale. The matter is made of elements and elements are made of atoms. Even the atoms of an element can be different, having a distinct number of protons and neutrons. This chapter covers the principles of atomic structure. You will learn what makes an atom and will be able to quantify the particles that make atoms. Perhaps more importantly, you will also learn about the periodic table of elements and the different types of chemical formulas.

2.1 The periodic table

The periodic table (see Figure 2.1) is a chart containing all known elements arranged in increasing number of electrons per atom in a way that elements with similar chemical and physical properties are located together. The periodic table contains all existing elements—some of them are synthetic others are natural—that form the matter arranged in columns and rows. Every element has a different name accompanied by a symbol that represents its name. The tabular arrangement of elements in the form of rows and columns allows further classification of the elements according to their properties. This section will cover the different features of the periodic table.

Elements and Symbols Elements cannot be broken down into simpler substances. For example, aluminum is an element only made of aluminum atoms and if you analyze the composition of a piece of this metal you would only find aluminum atoms. Chemical symbols are one- or two-letter abbreviations that represent the names of the elements. Only the first letter is capitalized and if a second letter exists in the element's name, the second letter should be lowercase. For example, the chemical symbol for aluminum is Al, written as capital A and lowercase l.

Sample Problem 15

Give the symbol or name the following elements: C, Oxygen, N, Phosphorus, Au, Iron, Na and Iodine.

SOLUTION

The name of the element with symbol C is carbon, whereas the chemical symbol of oxygen is O. Similarly, N stands for nitrogen, whereas the chemical symbol of Phosphorus is P. The chemical symbol of Au is Gold. The chemical symbol



of Iron is Fe and the chemical symbol of Iodine is I.

STUDY CHECK

Give the symbol or name the following elements: Ni.

Periods and groups The periodic table (see Figure 2.1) contains all elements arranged in rows and columns. The horizontal rows are called *periods* and the vertical columns are called *groups or families*. For example, the first period contains hydrogen (H) and helium (He), whereas the second group contains Beryllium (Be), Magnesium (Mg), Calcium (Ca), Strontium (Sr), Barium (Ba) and Radium (Ra). There are seven periods (periods 1-7) and 18 groups. Some of the groups are labeled with an A (e.g. group 8A) whereas others are labeled with a B (e.g. group 8B). Group numbers can be found written with roman numbers and a letter (A or B) or with a more modern group numbering of 1-18 going across the periodic table. For example, group 2 (Mg-Ra) can also be called IIA, and group 13 (B-Ti) is also known as IIIA.

Properties in the periodic table The physical and chemical properties of some elements of the table (see Figure 2.1) are similar, and these similarities led to the organization of the periodic table. Elements in the same group share properties and for example, oxygen and sulfur have similar properties: both are reactive elements. Differently, the properties across periods change going from metals to nonmetals. For example, the properties of Li and Ne are very different, and lithium is a reactive metal whereas neon is a nonreactive gas.

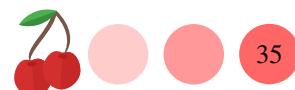
Metals, Nonmetals, and Metalloids Overall, the elements of the periodic table (see Figure 2.1) can be classified as metals, nonmetals, and metalloids. Metals are those elements on the left of the table and nonmetals are the elements on the right of the table. The elements between metals and nonmetals are called metalloids and include only B, Si, Ge, As, Sb, Te, Po, and At. Metals are shiny solids and usually melt at higher temperatures. Some examples of metals are Gold (Au) or Iron (Fe). Nonmetals are often poor conductors of heat and electricity with low melting points. They also tend to be matt (non-shiny), malleable, or ductile. Some examples of nonmetals are Carbon (C) or Nitrogen (N). Metalloids are elements that share some properties with metals and others with nonmetals. For example, they are better conductors of heat and electricity than nonmetals, but not as good conductors as metals. Metalloids are semiconductors because they can act as both conductors and insulators under certain conditions. An example of metalloids is Silicon (Si) which should not be confused with silicone, a chemical employed in prosthetics.

Sample Problem 16

Answer the following questions: (a) Give the group and period of the following elements, and give the name: Ca, Ir, and C. (b) Classify as alkali metal, alkali earth metal, transition metal, halogen or noble gas, and give the name: Mg, Li, Co, He, F. (c) Classify as metal, nonmetal or metalloid, and give the name: Ba, N, Si.

SOLUTION

(a)The period and group of Ca (Calcium) is 2 (2A) and 4, respectively. The period and group of Ir (Iridium) is 9 (8B) and 6, respectively. The period and group of C (Carbon) is 14 (IVA) and 2, respectively. (b) Mg (Magnesium) is an alkali earth metal, whereas Li (Lithium) is a alkali metal. Co (Cobalt) is a



transition metal. He (Helium) is a noble gas. F (Fluorine) is an halogen. (c) Ba (Barium) is a metal. N (Nitrogen) is a nonmetal. Si (Silicon) is a metalloid.

STUDY CHECK

Answer the following questions: (a) Give the group and period of the following elements, and give the name: Cl. (b) Classify as alkali metal, alkali earth metal, transition metal, halogen or noble gas, and give the name: Ne. (c) Classify as metal, nonmetal or metalloid, and give the name: W.

Classification of elements in terms of groups Some of the groups in the periodic table (see Figure 2.1) have specific names such as alkali metals, alkaline earth metals, transition metals, chalcogens, halogens, or noble gases. Alkali metals are the group 1A elements: lithium (Li), sodium (Na), potassium (K), rubidium (Rb), cesium (Cs), and francium (Fr). Alkali elements are soft and shiny metals, and they are also good conductors of heat and electricity, with low melting points. Alkali earth metals are group 2A (2) elements: beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba), and radium (Ra). Transition metals are the elements from groups 3 to 12 and they are located in the middle of the table. Chalcogens are group 6A (16) elements: oxygen (O), sulfur (S), selenium (Se), tellurium (Te), and polonium (Po). Halogens are group 7A (17) elements: fluorine (F), chlorine (Cl), bromine (Br), iodine (I), and astatine (At). Halogens are very reactive elements. Finally, noble gases are group 8A (18) elements: helium (He), neon (Ne), argon (Ar), krypton (Kr), xenon (Xe), and radon (Rn). They are inert and rarely combine with other elements in the periodic table, like a noble family: have you ever met a royal?

1 IA		Periodic Table of Elements																		18 VIIIA																			
1	1 1.0079 H Hydrogen	2 IIA		Alkali Metal		Alkaline Earth Metal		Transition metals		Metalloid		Chalcogen		Halogen		Noble Gas		Lanthanide/Actinide		Symbol		Name		z mass															
2	3 6.941 Li Lithium	4 9.0122 Be Beryllium																	5 10.811 B Boron	13 IIIA	6 12.011 C Carbon	14 IVA	7 14.007 N Nitrogen	8 15.999 O Oxygen	9 18.998 F Fluorine	10 20.180 Ne Neon													
3	11 22.990 Na Sodium	12 24.305 Mg Magnesium			3 IIIB	4 IVB	5 VB	6 VIB	7 VIIIB	8 VIIIIB	9 VIIIIB	10 VIIIIB	11 IB	12 IIB				15 26.982 Al Aluminium	16 30.974 Si Silicon	17 32.065 P Phosphorus	18 39.948 S Sulphur	19 40.078 Ca Calcium	20 40.078 K Potassium	21 44.956 Sc Scandium	22 47.867 Ti Titanium	23 50.942 V Vanadium	24 51.996 Cr Chromium	25 54.938 Mn Manganese	26 55.845 Fe Iron	27 58.935 Co Cobalt	28 58.693 Ni Nickel	29 63.546 Cu Copper	30 65.539 Zn Zinc	31 69.723 Ga Gallium	32 72.64 Ge Germanium	33 74.922 As Arsenic	34 78.96 Se Selenium	35 79.904 Br Bromine	36 83.8 Kr Krypton
4	19 39.098 K Potassium	20 40.078 Ca Calcium			21 44.956 Sc Scandium	22 47.867 Ti Titanium	23 50.942 V Vanadium	24 51.996 Cr Chromium	25 54.938 Mn Manganese	26 55.845 Fe Iron	27 58.935 Co Cobalt	28 58.693 Ni Nickel	29 63.546 Cu Copper	30 65.539 Zn Zinc				31 69.723 Ga Gallium	32 72.64 Ge Germanium	33 74.922 As Arsenic	34 78.96 Se Selenium	35 79.904 Br Bromine	36 83.8 Kr Krypton																
5	37 85.468 Rb Rubidium	38 87.62 Sr Strontium			39 88.906 Y Yttrium	40 91.224 Zr Zirconium	41 92.906 Nb Niobium	42 95.94 Mo Molybdenum	43 96 Tc Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.42 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium				49 114.82 In Indium	50 118.71 Sn Tin	51 121.76 Sb Antimony	52 127.6 Te Tellurium	53 126.9 I Iodine	54 131.29 Xe Xenon																
6	55 132.91 Cs Cesium	56 137.53 Ba Barium			57-71 La-Lu Lanthanide	72 178.49 Hf Hafnium	73 180.95 Ta Tantalum	74 183.84 W Tungsten	75 186.21 Re Rhenium	76 190.23 Os Osmium	77 192.22 Ir Iridium	78 195.08 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury				81 204.38 Tl Thallium	82 207.2 Pb Lead	83 208.98 Bi Bismuth	84 209 Po Polonium	85 210 At Astatine	86 222 Rn Radon																
7	87 225 Fr Francium	88 226 Ra Radium			89-103 Ac-Lr Actinide	104 261 Rf Rutherfordium	105 262 Db Dubnium	106 266 Sg Seaborgium	107 264 Bh Bohrium	108 277 Hs Hassium	109 268 Mt Meitnerium	110 281 Ds Darmstadtium	111 280 Rg Roentgenium	112 285 Ub Ununbium				113 284 Uut Ununtrium	114 289 Uuq Ununquadium	115 288 Uup Ununpentupm	116 293 Uuh Ununhexium	117 292 Uus Ununseptium	118 294 Uuo Ununoctium																
					57 138.91 La Lanthanum	58 140.12 Ce Cerium	59 140.91 Pr Praseodymium	60 144.24 Nd Neodymium	61 145 Pm Promethium	62 150.36 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.95 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.04 Yb Ytterbium	71 174.97 Lu Lutetium																				
					89 227 Ac Actinium	90 232.04 Th Thorium	91 251.04 Pa Protactinium	92 258.05 U Uranium	93 257 Np Neptunium	94 244 Pu Plutonium	95 245 Am Americium	96 247 Cm Curium	97 247 Bk Berkelium	98 251 Cf Californium	99 252 Es Einsteinium	100 257 Fm Fermium	101 258 Md Mendelevium	102 259 No Neptunium	103 262 Lr Lawrencium																				

Figure 2.1 The periodic table of the elements

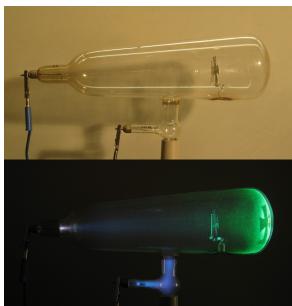
How to classify Hydrogen At first sight, hydrogen (H) may seem to be put in the wrong spot on the periodic table (see Figure 2.1). Although it is located at the top of Group 1A (1), it is not an alkali metal, as it has very different properties. Thus hydrogen does not belong to the alkali metals, being nonmetal.



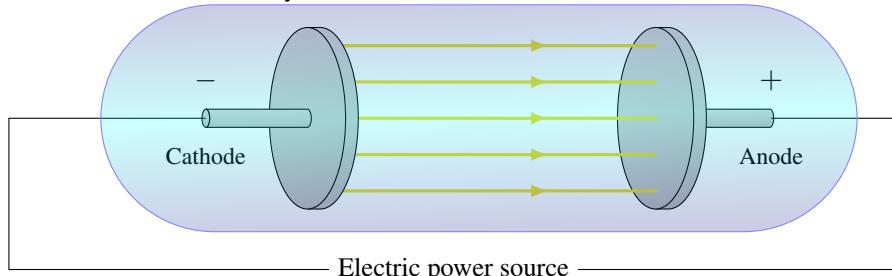
2.2 Early experiments of the atom

Scientists wondered about the nature of the atom and its structure for years. In a series of experiments carried out in the late nineteenth century, scientists such as J.J. Thomson, Henri Becquerel, and Ernest Rutherford gained insight into the nature and structure of the atom. These remarkable scientists and these creative experiments helped shape the view of the atom that we have nowadays.

▼A cathode tube



© www.wallpaperflare.com



▼Millikan's apparatus



© www.wallpaperflare.com

▼A plum pudding, with the electrons represented by the raisins



© wikipedia

Figure 2.2 Cathode-ray tube made of two electrodes and a partially evacuated gas tube. The electrons, generated on the negatively charged electrode names cathode, excite the gas in the tube generating glow.

Charge to mass ratio of an electron The English researcher J.J. Thomson investigated electric discharges in partially evacuated tubes—tubes in which the air has been partially removed (See Figure 2.2); these tubes, made of a positive and negative electrode, are the base of old-fashion, bulky televisions. Thomson found that rays emanated from the negative electrode when applying high-voltage to these tubes. These rays were named cathodic rays as the negative electrode of the tube is called the cathode. Thomson also found that cathodic rays were repelled from the negative pole of an electric field. Hence, these rays were postulated to be a stream of negatively charged particles, now known as electrons. By studying the deflection of these rays by an electric field, Thomson was able to calculate the charge-to-mass ratio of an electron:

$$\frac{e}{m_e} = -1.76 \times 10^8 \text{ C/g} \quad (2.1)$$

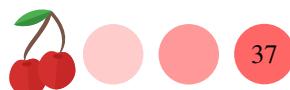
where:

e is the charge of an electron

m_e is the mass of an electron

Overall, the biggest of Thomson's discoveries was that all atoms are made of negatively charged particles. As atoms are charge-neutral, they are also made of positively charged particles. These observations led to a new atomic model, the *plum pudding model*, that envisioned atoms as a diffuse cloud of positive charges with negative electrons embedded in it. The name plum pudding comes from an English dessert that contains a raising spread. A different scientist, Robert Millikan, revealed the magnitude of the electric charge of the electron. Millikan used an apparatus that dispersed charged oil droplets falling under the influence of an electric field. Given the applied voltage and the droplet mass, Millikan was able to calculate the droplet charge. He found that the oil drop charge was always a whole number times the electron charge,

$$e = 1.60 \times 10^{-19} \text{ C} \quad (2.2)$$



where a Coulomb is a unit of charge. With the value of the charge-to-mass ratio of an electron and the electron charge, Millikan was also able to calculate the mass of an electron,

$$m_e = 9.11 \times 10^{-31} \text{ kg.} \quad (2.3)$$

The atom nucleus Ernest Rutherford carried out further experiments to validate the plum pudding model of the atom. He exposed a thin sheet of metal foil to α particles known to be massive and positively charged particles. According to the plum pudding model, the bulky α particles should have crashed through the thin foil and traversed through without being deflected. However, the results did not corroborate his expectations. Indeed, some particles traversed the film, whereas others were slightly deflected and some were strongly deflected at large angles. These observations did not corroborate the plum pudding model. However, they contributed to the creation of the modern atomic model in which a large number of positive charges were concentrated at a point—called the nucleus—instead of being spread whereas the electrons move around the nucleus at large distances from it. The figure below represents the experiment carried out by Rutherford in which alpha particles were scattered on a thin field made of gold.

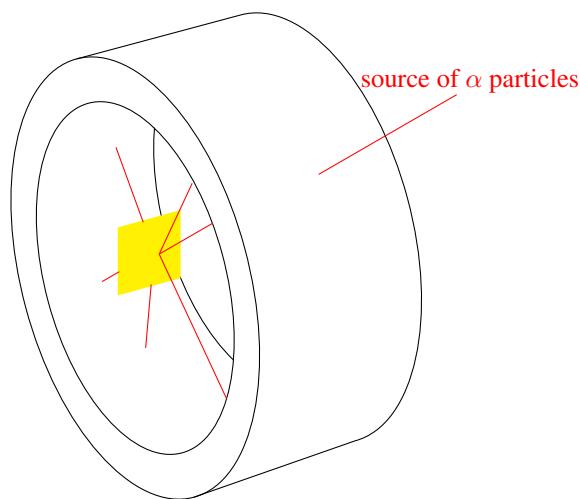


Figure 2.3 Rutherford's scattering: the elastic scattering of charged particles by the Coulomb interaction after a particle beam passed through a thin gold foil obstruction.

Radiation In the last part of the nineteenth century, scientists came to the discovery that some materials were able to produce high-energy radiation. Among the scientist working in this field, Henri Becquerel discovered that pitchblende, a mineral containing uranium, was able to produce an image on a photographic plate in the absence of light. In the early twentieth century, three different types of radiation were discovered: alpha radiation, beta radiation, and gamma radiation. Further studies revealed that gamma radiation was made of gamma particles, high-energy radiation, whereas beta radiation was made of high-energy electrons. Alpha particles were found to be positively charged, with a charge twice the charge of an electron and a mass 7300 times that of the electron. These particles were indeed Helium's nucleus, resulting from removing electrons from atoms of Helium.

2.3 The atom

Atoms are the smallest piece of an element that retains their characteristics. They are the building blocks of matter. This section covers the structure of the atom. You will learn how



to calculate the number of subatomic particles that made an atom and how to differentiate atoms of an element—all atoms of an element are not equal.

Atomic Structure An atom is an electrically neutral, spherical entity made of a nucleus surrounded by negatively charged electrons. Atoms contain three atomic particles: the proton, neutron, and electron. Protons have a positive charge (+), whereas electrons carry a negative charge (−). Both electrons and protons have the same charge in magnitude but with opposite signs. Neutrons on the other hand are neutral, and they have no electrical charge. Protons and neutrons are located in the core of the atom, which is called the nucleus, and account for the mass of the atom. The only exception is the hydrogen atom, the smallest element, with just one proton in the nucleus. Electrons are delocalized in the exterior part of the atoms. They are not necessarily located in a specific spot and their existence spreads in the area next to the nucleus. Electrons move rapidly and are spread and held by nuclear attraction. Atoms are neutral without a charge as the number of electrons and protons are the same. Some atoms have a positive charge, resulting in removing electrons, and we call these cations. Others—called anions—can have a negative charge as a result of accepting a negatively charged electron. The mass of a proton or neutron is 2000 times larger than the mass of an electron and the atom's diameter is more than 10000 times the diameter of its nucleus. The nucleus is very dense being 99% of an atom's mass while occupying a small volume.

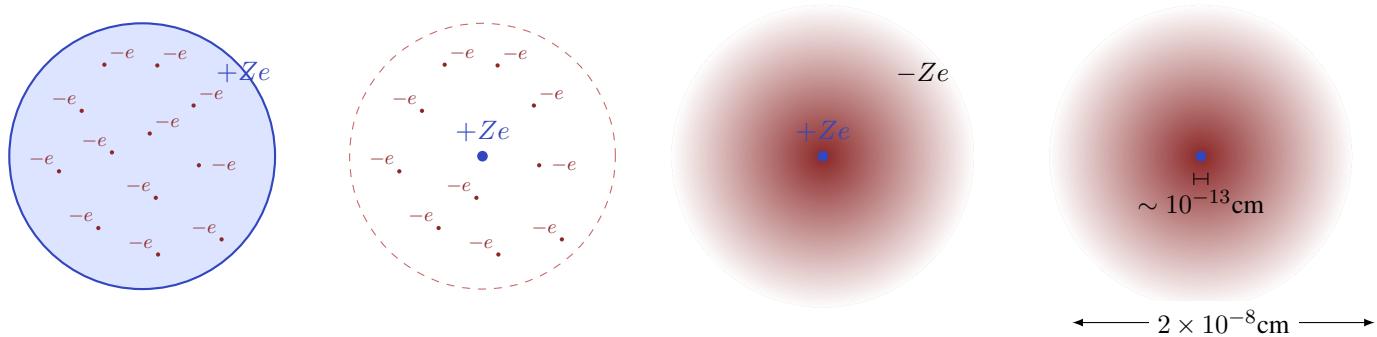
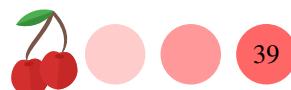


Figure 2.4 Three models of the atom. From left to right: the plum pudding model, the updated plum pudding model according to Rutherford's observations, (two right images) the modern atomic model. Z is the atomic number of the atom.

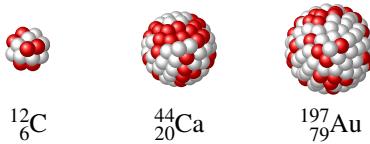
Elements are made of atoms, and each atom of an element is characterized by an atomic number (Z) and a mass number (A). The atomic number (Z) of an element indicates the number of protons in an atom. This number can be easily located in the periodic table (see Figure 2.1). All atoms of an element have the same atomic number, whereas the atomic number of different elements differ. For example, Carbon has an atomic number of $Z=6$, whereas Oxygen has an atomic number of $Z=8$. The mass number (A) of an element indicates the combined number of protons and neutrons. Mass numbers can not be found in the periodic table. More importantly, different atoms of the same element can have different mass numbers. For example, a Carbon atom made of 6 neutrons and 6 protons has a mass number of $A=12$. Both A and Z for an atom X are indicated in the following form called isotope notation:

$$\text{Atomic and mass number } {}^A_Z \text{X}$$

As an example, the notation ${}^{24}_{12} \text{Mg}$ means that the atomic number of Mg is $Z=12$ and the mass number is $A=24$. Using the isotope notation, one can quickly identify the



number of protons, neutrons, and electrons in an atom. As the atomic number is always indicated on the bottom part (e.g. Mg has 12 electrons). At the same time, the number of electrons and protons in a neutral atom is the same—neutral means an atom without a charge. The number of neutrons of an isotope can be computed by subtracting the atomic number from the mass number. Below you can find three different atoms, an atom of Carbon with 12 protons and neutrons, a larger atom of Calcium with 44 protons and neutrons, and an even larger atom of Gold with 197 protons and neutrons.



Sample Problem 17

Calculate the number of protons, neutrons and electrons of the following atoms:

- (a) $^{27}_{12}\text{Mg}$ (b) $^{22}_{10}\text{Ne}$ (c) $^{20}_{10}\text{Ne}$

SOLUTION

- (a) $^{27}_{12}\text{Mg}$ has 12 electrons ($Z=12$) and 12 protons as well (the number of electrons and protons are the same if the atom is neutral), and 15 neutrons, as $27-12=15$.
 (b) $^{22}_{10}\text{Ne}$ has 10 electrons and 10 protons, and 12 neutrons. (c) $^{20}_{10}\text{Ne}$ has 10 electrons and 10 protons, and 10 neutrons as well.

◆ STUDY CHECK

Calculate the number of protons, neutrons and electrons of the following atoms:

- (a) $^{32}_{16}\text{S}$ (b) $^{34}_{16}\text{S}$ (c) $^{36}_{16}\text{S}$

Isotopes All atoms of an element have the same atomic number but may differ in terms of mass number. Isotopes are atoms of the same element with different numbers of neutrons and therefore with different mass numbers but with the same atomic number. For example: $^{24}_{12}\text{Mg}$, $^{25}_{12}\text{Mg}$ and $^{26}_{12}\text{Mg}$ are three isotopes of Mg. $^{27}_{12}\text{Mg}$ is heavier than $^{24}_{12}\text{Mg}$ as it contains more neutrons and protons in the nucleus. Most elements occur in nature in a particular isotopic composition, and each of the isotopes has a specific proportional abundance. For example, the abundance of $^{24}_{12}\text{Mg}$ is 79%, and the abundance of $^{25}_{12}\text{Mg}$ and $^{26}_{12}\text{Mg}$ is 10% and 11%, respectively. This means, $^{24}_{12}\text{Mg}$ is more abundant than for example $^{26}_{12}\text{Mg}$.



Another example of isotopes can be found in Carbon, with two naturally occurring isotopes. In the case of charged atoms, we have the cations have fewer electrons than their corresponding atom, whereas anions have more electrons, both based on their charge. The mass of an atom is measured relative to the mass of an atomic standard, the Carbon-12 atom, whose mass is defined as 12 atomic units of mass, amu. For example, the mass of ^1H is 1.008 amus. The term atomic unit of mass has been renamed to dalton (Da). Therefore, the mass of ^1H is 1.008 amus or 1.008 Da. The atomic mass is a relative unit of mass equivalent to $1.66054 \times 10^{24}\text{g}$.

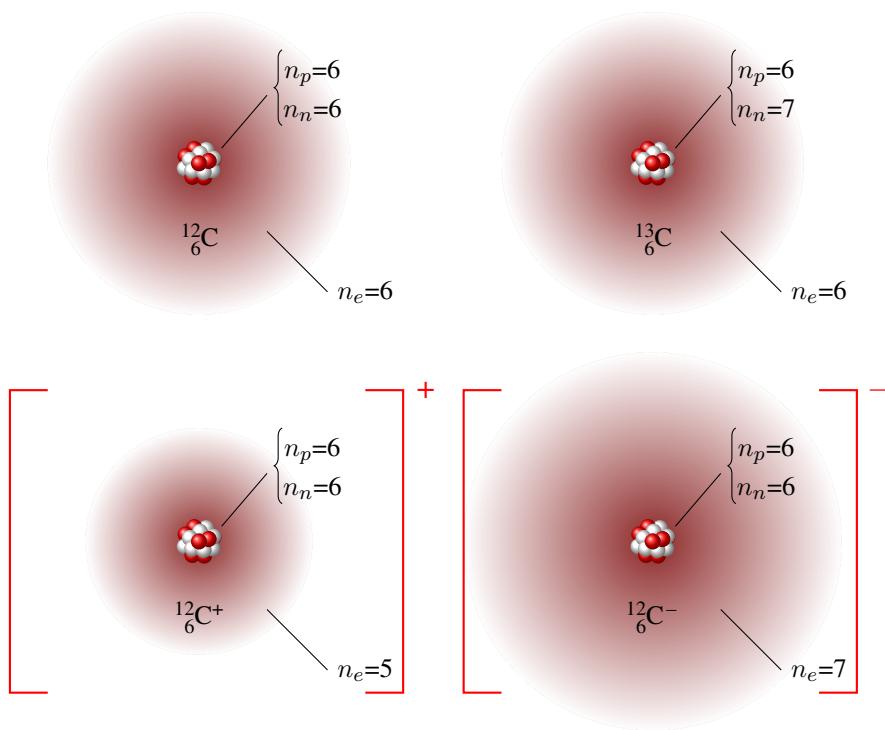


Figure 2.5 Representations of four different atoms, two neutral atoms on top and two ions on the bottom.

Average atomic mass As atoms are made of numerous isotopes—this means different atoms of the same element but with a different number of neutrons and hence different weights. The average atomic mass (also called atomic weight) represents the mass of the atoms of an element and results from all existing isotopes taking into account their abundance. It is the average of the masses of the naturally occurring isotope weighted according to their abundance expressed in atomic mass units or daltons. We can think of *% relative abundance*, and for example, the *% relative abundance* of ^1H is 99%. But we can also think of *fractional abundance*, that in the case of ^1H would be 0.99. For an element with n isotopes each with different masses (A_1, A_2, \dots, A_n) and different fractional abundances (f_1, f_2, \dots, f_n), the atomic mass is given by

$$\text{Atomic mass} = \sum_{i=1}^n A_i \cdot f_i = A_1 \cdot f_1 + A_2 \cdot f_2 + \dots + A_n \cdot f_n$$

Note that when adding the fractional abundances of all isotopes, one should obtain a value of one:

$$\sum_{i=1}^n f_i = f_1 + f_2 + \dots + f_n = 1$$

Atomic masses can be simply found in any periodic table (see Figure 2.1) for each element. For example, the atomic mass of oxygen (O) is 15.999 amu and the atomic mass of nitrogen (N) is 14.007 amu. The atomic mass found in the periodic table is an average that results from including the mass of the different isotopes and their abundance. Table 2.1 lists the relative abundance of a series of common isotopes.

Sample Problem 18

Naturally occurring copper (Cu) consists of 69.17% ^{63}Cu and 30.83% ^{65}Cu . The mass of ^{63}Cu is 62.939598 amu, and the mass of ^{65}Cu is 64.927793 amu.

What is the atomic mass of copper?

SOLUTION

The weighted average is the sum of the mass of each isotope times its fractional abundance. We have that the isotope ^{63}Cu has a mass of 62.939598 amu and an abundance of 69.17%, that is the same as 0.6917. At the same time, the isotope ^{65}Cu has a mass of 64.927793 amu and an abundance of 0.3083. After adding both contributions, we have:

$$62.939598 \text{ amu} \times \frac{69.17}{100} + 64.927793 \text{ amu} \times \frac{30.83}{100} = 63.55 \text{ amu}$$

We can use the table below to obtain the final result:

Isotope	m_i (amu)	f_i	$m_i \times f_i$
^{63}Cu	62.939598	0.6917	43.53
^{65}Cu	64.927793	0.3083	20.02
Average atomic mass (amu)			$= \sum m_i \times f_i = 63.55$

◆ STUDY CHECK

Lithium is made up of two isotopes, Li-7 (7.016003 amu) and Li-6 (6.015121 amu). Calculate the percent abundance of each isotope knowing that lithium's atomic weight is 6.94 amu.

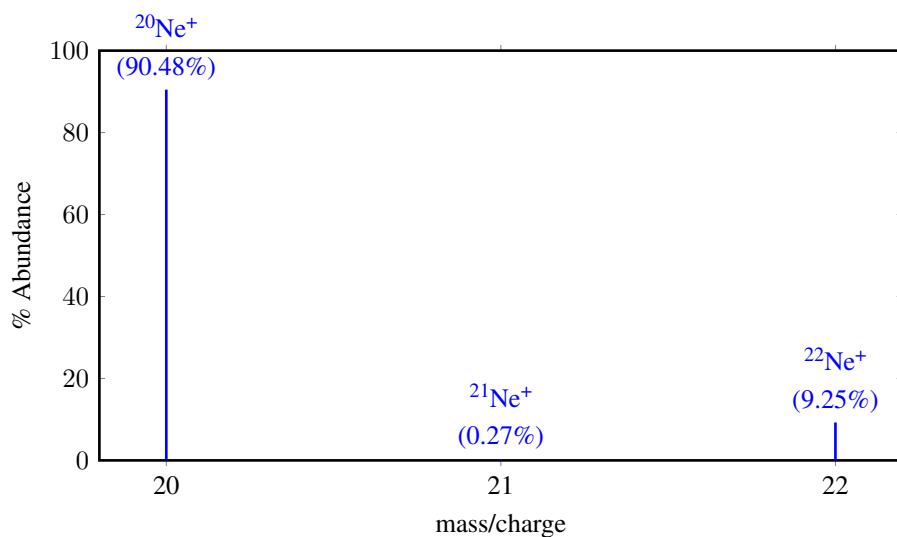


Figure 2.6 Mass spectra of Neon with three peaks corresponding to three different isotopes with different relative abundance.

Mass spectrometry Mass spectroscopy is a technique used to determine the isotopic composition of an element. With this technique, we can measure the relative mass and abundance of small atomic particles. In this technique, high-energy electrons collide with atoms or molecules to form ionized atoms. For example, if Ne would be analyzed, high energy electrons would produce Ne^+ characterized by its mass charge ratio, m/e . Different isotopes would have different m/e ratios. The positively charged



particles produced after the impact would be attracted toward a series of negatively charged plates with slits in them. Some of these particles would pass through the slits into an evacuated tube exposed to the effect of a magnetic field. As the particles enter the evacuated region their paths are bent so that the lightest particles (low m/e) are more deflected than the heaviest particles (high m/e). Finally, the particles would stick to a detector recording their relative position and abundance. The spectrometer also provided the mass ratio of an isotope with respect to the mass standard, ^{12}C .

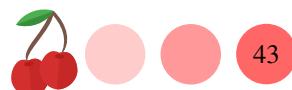
Table 2.1 Isotope abundance of some elements

Element	Isotope	% Abundance	Element	Isotope	% Abundance
Hydrogen	^1H	99.9885%	Silicon	^{28}Si	92.2297%
	^2H	0.0115%		^{29}Si	4.6832%
Helium	^3He	0.000137%	Sulfur	^{30}Si	3.0872%
	^4He	99.999863%		^{32}S	94.93%
Lithium	^6Li	7.59%	Chlorine	^{33}S	0.76%
	^7Li	92.41%		^{34}S	4.29%
Boron	^{10}B	19.9%	Argon	^{36}S	0.02%
	^{11}B	80.1%		^{35}Cl	75.78%
Carbon	^{12}C	98.93%	Potassium	^{37}Cl	24.22%
	^{13}C	1.07%		^{36}Ar	0.3365%
Nitrogen	^{14}N	99.632%	Potassium	^{38}Ar	0.0632%
	^{15}N	0.368%		^{40}Ar	99.6003%
Oxygen	^{16}O	99.757%	Potassium	^{39}K	93.2581%
	^{17}O	0.038%		^{40}K	0.0117%
	^{16}O	0.205%		^{41}K	6.7302%

2.4 An introduction to molecules

The periodic table (see Figure 2.1) contains all elements in nature. At the same time, elements combine to form molecules. For example, in the air there are traces of Argon—this is an element—and also water, a molecule (H_2O) that results from the combination of two elements, hydrogen (H) and oxygen (O). This section will first introduce some of the properties of molecules, without paying attention to their chemical names that will be covered in the following chapters.

Molecular weight Here are two examples of molecules: molecular oxygen O_2 and molecular nitrogen N_2 . How do we interpret these formulas? The subscript "2" indicates that each molecule contains two atoms. For example, a O_2 molecule is made of two oxygen atoms O. At the same time, the weight of a set of molecules is called the molecular weight (MW). However, you will find different terms to refer to the same property such as molecular mass, molar mass, or formula unit mass. All these terms indeed mean the weight of a large set of molecules. We can calculate the MW by adding the weight of each atom that forms the molecule taking into account the number of atoms of each element present in the molecule. The units of molecular weight are the same as the units of atomic weight: amu, atomic mass units.

**Sample Problem 19**

Calculate: (a) The atomic weight of O; (b) the molecular mass of molecular oxygen, O₂

SOLUTION

- (a) According to the periodic table the atomic weight (AW) of O is 15.999 amu.
 (b) The molar mass of O₂ is the result of adding the atomic masses of 2O atoms, that is 31.998 amu, close to 32 amu.

◆ STUDY CHECK

Calculate the molar mass of water H₂O and ammonia, NH₃

Mass percent composition of a compound Look at these two molecules: C₂H₂ and C₂H₆. They contain different amounts of hydrogen. We quantify the amount of an element in a compound using the mass % composition. The mass % of an element in a compound is the mass of the element concerning the molecular weight of the molecule in percent form. Mind that you have to take into account the molecular indexes in the compound as C₂H₂ is made of 2H and C₂H₆ is made of 6H. For example, given that the molar mass of C₂H₂ is 26 amu, the mass % of hydrogen in C₂H₂ would be:

$$\%_H \text{ in } C_2H_2 = \frac{2 \cdot AW(H)}{MW(C_2H_2)} \times 100 = \frac{2 \cdot 1}{26} \times 100 = 7.7\%$$

Similarly, the mass % of C would be:

$$\%_C \text{ in } C_2H_2 = \frac{2 \cdot AW(C)}{MW(C_2H_2)} \times 100 = \frac{2 \cdot 12}{26} \times 100 = 92.3\%$$

By adding the mass % of all elements in a molecule we should obtain 100.

$$\%_H \text{ in } C_2H_2 + \%_C \text{ in } C_2H_2 = 100$$

Sample Problem 20

Calculate the mass % composition for each element of glucose, C₆H₁₂O₆.

SOLUTION

We first need the molecular weight of glucose, C₆H₁₂O₆, that is: 6 · 12 + 12 · 1 + 6 · 16 = 180 amu. Now we can calculate the mass percent of carbon, hydrogen and oxygen:

$$\%_C \text{ in } C_6H_{12}O_6 = \frac{6 \cdot 12}{180} \times 100 = 40\%$$

$$\%_H \text{ in } C_6H_{12}O_6 = \frac{12 \cdot 1}{180} \times 100 = 6.6\%$$

By subtraction, we have that %_O in C₆H₁₂O₆ = 53.4.

◆ STUDY CHECK

Ureas CO(NH₂)₂ is a colorless crystalline compound excreted in urine, product of protein metabolism in mammals. Calculate the mass % composition for each element of urea.



There are two different types of formulas: molecular formulas and empirical formulas. Empirical formulas (EFs) are simplified formulas resulting from an experiment, whereas molecular formulas (MFs) are exact formulas of molecules. For example, the molecular formula of hydrogen peroxide, a mild antiseptic used on the skin to prevent infection of minor cuts, is H_2O_2 as the hydrogen peroxide molecule is made of two oxygen and two hydrogen atoms. Differently, the empirical formula of the same chemical is HO, being this the result of the simplification of H_2O_2 . One can obtain empirical formulas simply by dividing the molecular formula by the smallest integer number, of course, given you know the molecular formula. The word empirical means "from an experiment", and the use of empirical formulas comes from the fact that the formulas of all chemicals come from experiments, and from experiments, one normally can only obtain ratios of atomic composition.

Sample Problem 21

From the following formulas identify the empirical and molecular formulas:
 P_4O_{10} , $\text{C}_3\text{H}_6\text{O}$, N_2O_4 and C_5H_{11} .

SOLUTION

Empirical formulas are simplified versions of molecular formulas. For example, $\text{C}_3\text{H}_6\text{O}$ and C_5H_{11} are empirical formulas. Differently, P_4O_{10} and N_2O_4 are molecular formulas.

❖ STUDY CHECK

Given the following molecular formulas, obtain the corresponding empirical formula: P_4O_{10} , N_2O_4 and $\text{C}_6\text{H}_{18}\text{O}_3$.

Molecular weight of empirical formulas and molecular formulas

The molecular weight of an empirical formula and its corresponding molecular formula are related by the following formula:

$$n = \frac{MW_{MF}}{MW_{EF}}$$

where:

MW_{EF} is the molecular weight of the empirical formula

MW_{MF} is the molecular weight of the molecular formula

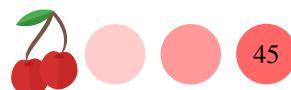
n is an integer number such as 1, 2, 3...

Understanding the formula above is simple. On one hand, the MW of a molecular formula H_2O_2 is 34 amu. On the other hand, the molecular weight of the empirical formula of the same chemical HO is 17 amu. If we do 34/17 we would obtain 2, as we need to multiply HO by two to obtain H_2O_2 . As a final note, mind that empirical formulas are just simplified formulas. So when we think about the molecular weight of a chemical we normally have a molecular formula in mind. Let us work on an example.

Sample Problem 22

Given that the empirical formula of dichloroethane is ClCH_2 and the molecular weight of the chemical is 98 amu, calculate the molecular formula of dichloroethane.

SOLUTION



Given the empirical formula of dichloroethane one can think of many different molecular formulas, for example: $\text{Cl}_3\text{C}_3\text{H}_6$ or $\text{Cl}_2\text{C}_2\text{H}_4$. From these, and many other, there is only one real molecular formula. How do we calculate the real molecular formula? By comparing the MW of the molecular and empirical formula we can figure out the number of time we need to multiply the MF to obtain the EF. We know the MW is 98amu. Using the EF we can also calculate a MW: $35 + 12 + 2 \cdot 1 = 49$ amu. If we compare both number using the formula:

$$n = \frac{MW_{MF}}{MW_{EF}}$$

we have: $n = 98/49$ and solving we have $n = 2$. Therefore the MF is: $\text{Cl}_2\text{C}_2\text{H}_4$.

STUDY CHECK

The empirical formula of dinitrogen tetroxide, a red-brown liquid with an unpleasant chemical odor, is NO_2 and the molecular weight of the chemical is 92 amu. Calculate the molecular formula of dinitrogen tetroxide.

2.6 Determining empirical formulas

We said that the formula of a chemical that takes into account the correct number of atoms in a molecule is the molecular formula and therefore the real molecular weight of a chemical comes from these formulas. Empirical formulas are obtained from experiments in which a chemical is fragmented and analyzed so that the elements in the molecule and the mass percentage of each element are determined. Molecular formulas are obtained by using the molecular weight of the chemical and the empirical formula. Mind that the formula of a chemical that takes into account the correct number of atoms in a molecule is the molecular formula and therefore the real molecular weight of a chemical comes from these formulas. Let us work on an example to learn the procedure of obtaining molecular formulas.

Calculating molecular formulas We want to calculate the empirical formula of a chemical given that the chemical contains 2.8 g of nitrogen and 6.4 g of oxygen. To calculate the EF we will set up a table like the one presented below.

Empirical Formula Calculation		
	N	O
Grams	2.8g	6.4g
AW	14	16
Grams/AW	0.2	0.4
÷ by smallest	1	2
Formula	$\text{N}_1\text{O}_2=\text{NO}_2$	

In each column, we will add each of the elements that form the molecule. In the first row, we will include the grams of each element (sometimes this information is given in terms of mass %), in the second we will divide the grams of each element by its atomic



weight (AW(N)=14amu, AW(O)=16amu). Among all numbers of the second row (in this example 0.2 and 0.4), we will select the smallest number (0.2). Once we have the smallest, we will divide all numbers by the smallest, and that will give us round numbers (1 and 2); these will be the numbers in an empirical formula: NO_2 .

Sample Problem 23

The mass percentage composition of a compound is: 18.59% O, 37.25% S, and 44.16% F. Calculate its empirical formula.

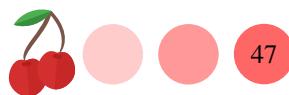
SOLUTION

We will set up the the molecular formula table, knowing that the percentage are mass percentages, that is the mass of each element in the chemical, hence they should go in the grams row. Also the atomic weights of O, S and F are 16, 32 and 19 amu.

Empirical Formula Calculation			
	O	S	F
Grams	0.1859g	0.3725g	0.4416g
AW	16	32	19
Grams/AW	0.0116	0.0116	0.0232
÷ by smallest	1	1	2
Formula	OSF_2		

◆ STUDY CHECK

What is the empirical formula of a compound if a sample contains 10.28 g of C, 1.71 H and 12.71 g of oxygen?



CHAPTER 2

THE PERIODIC TABLE

2.1 Select from below the atomic symbol for the element Gold is: (a) Go (b) Au (c) G (d) Ca (e) Ol

2.2 Select from below the atomic symbol for the element Calcium is: (a) Go (b) Au (c) G (d) Ca (e) Ol

2.3 The atomic symbol for aluminum is: (a) Al (b) Am (c) A (d) Sn (e) Ag

2.4 The atomic symbol for iron is: (a) Ir (b) Fs (c) Fe (d) In (e) Ir

2.5 Ca is the symbol for: (a) Carbon (b) Calcium (c) Cobalt (d) Copper (e) Cadmium

2.6 Write down the symbol for the following elements:
(a) Magnesium (b) Manganese (c) Mercury (d) Molybdenum
(e) Neodymium (f) Neon (g) Neptunium (h) Nickel
(i) Osmium (j) Palladium

2.7 Write down the symbol for the following elements:
(a) Phosphorus (b) Platinum (c) Plutonium (d) Polonium
(e) Potassium (f) Radium (g) Radon (h) Rhenium
(i) Rhodium (j) Rubidium (k) Ruthenium

2.8 Write down the element names for the following chemical symbols: (a) Sc (b) Se (c) Si (d) Ag (e) Na (f) Sr (g) S (h) Te

2.9 Write down the element names for the following chemical symbols: (a) Tl (b) Th (c) Sn (d) Ti (e) W (f) U (g) V (h) Xe (i) Zn (j) Zr

2.10 Which of the following elements is a metal? (a) Nitrogen (b) Lithium (c) Calcium (d) Iron (e) Iodine

2.11 Which of the following elements is a nonmetal?
(a) Nitrogen (b) Lithium (c) Calcium (d) Iron (e) Iodine

2.12 Which of the following elements is a alkali metal?
(a) Nitrogen (b) Lithium (c) Calcium (d) Iron (e) Ruthenium

2.13 Which of the following elements is a alkaline earth metal? (a) Nitrogen (b) Lithium (c) Calcium (d) Iron (e) Ruthenium

2.14 Which of the following elements is a halogen?
(a) Nitrogen (b) Lithium (c) Calcium (d) Iron (e) Iodine

2.15 Which of the following elements is a chalcogen?
(a) Oxygen (b) Lithium (c) Calcium (d) Iron (e) Iodine

2.16 What is the symbol of the element in Period 4 and Group 2? (a) Be (b) Mg (c) Ca (d) C (e) Si

2.17 What is the symbol of the element in Period 2 and Group 2? (a) Be (b) Mg (c) Ca (d) C (e) Si

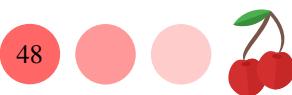
2.18 Identify the group number described by: (a) Starts with Zn (b) Ends with Ra (c) Contains the elements O, S, and Se (d) Is located to the right of Mn (e) Is located to the left of Ti

2.19 Identify the group number described by: (a) Starts with B (b) Ends with Rn (c) Contains the elements Mn, Tc, and Re (d) Is located to the right of H (e) Is located to the left of F

2.20 Identify the elements located at: (a) group 7A and period 3 (b) An halogen at period 5 (c) An alkaline earth at period 7 (d) An alkali at period 3

2.21 Identify the elements located at: (a) group 2A and period 4 (b) An halogen at period 3 (c) An alkaline earth at period 5 (d) An alkali at period 6

2.22 Identify the elements below as metal, nonmetal or metalloid: (a) B (b) Sb (c) Fe (d) Zn (e) H



2.23 Identify the elements below as metal, nonmetal or metalloid: (a) A shiny element (b) C (c) A electrically conducting element (d) A dull element (e) A semiconductor

EARLY EXPERIMENTS OF THE ATOM

2.24 From the following scientist, J.J. Thomson, Robert Millikan, Henri Becquerel, and Ernest Rutherford, indicate who: (a) Discovered the element Uranium in a mineral (b) Scattered atoms on helium on a gold thin layer (c) Unsuccessfully validated the plum pudding model

2.25 From the following scientist, J.J. Thomson, Robert Millikan, Henri Becquerel, and Ernest Rutherford, indicate who: (a) Worked with cathodic rays (b) Calculate the charge-to-mass ratio of the electron (c) Worked with oil drops to calculate the electric charge of the electron

2.26 Based on Rutherford's experiment, answer the following: (a) What did Rutherford expect after aiming particles to the gold foil? (b) What did Rutherford found after aiming particles to the gold foil?

2.27 Rutherford's scattering experiment was based on: (a) The scattering of alpha particles from gold foil (b) The scattering of beta particles from gold foil (c) The scattering of alpha particles from zinc foil (d) The scattering of gamma particles from iron foil

THE ATOM

2.28 In an atom, the nucleus contains: (a) an equal number of protons and electrons. (b) all the protons and neutrons (c) all the protons and electrons (d) only neutrons (e) only protons

2.29 In an ion, the nucleus contains: (a) an equal number of protons and electrons. (b) all the protons and neutrons (c) all the protons and electrons (d) only neutrons (e) only protons

2.30 Associate the following statements with either an electron, a proton or a neutron: (a) are found away from the nucleus (b) are attracted to a proton (c) are negatively charged (d) are found in the nucleus

2.31 Associate the following statements with either an electron, a proton or a neutron: (a) are attracted to an electron (b) have the smallest mass (c) are positively charged (d) are neutrally charged

2.32 Indicate whether the following statements are true or false: (a) Neutrons repel to each other (b) Protons and neutrons have opposite charges (c) Electrons repel to each other

2.33 Indicate whether the following statements are true or false: (a) Protons and electrons have opposite charges (b) Protons repel to each other (c) Neutrons and protons have very different mass

2.34 The atomic number of an atom is equal to the number of: (a) nuclei (b) neutrons (c) neutrons plus protons (d) electrons plus protons (e) electrons

2.35 The mass number of an atom is equal to the number of: (a) nuclei (b) neutrons (c) neutrons plus protons (d) electrons plus protons (e) electrons

2.36 Consider a neutral atom with 30 protons and 34 neutrons. The atomic number of the element is: (a) 30 (b) 32 (c) 34 (d) 64 (e) 94

2.37 Consider a neutral atom with 40 protons and 45 neutrons. The mass number of the element is: (a) 40 (b) 45 (c) 80 (d) 85 (e) 94

2.38 Identify the name of the following isotopes (a) $^{106}_{44}X$ (b) $^{93}_{40}X$ (c) $^{85}_{36}X$

2.39 Identify the name of the following isotopes (a) $^{155}_{63}X$ (b) $^{126}_{50}X$ (c) $^{107}_{46}X$

2.40 Select the isotopes from the list below: (a) $^{90}_{228}X$ (b) $^{231}_{90}X$ (c) $^{230}_{90}X$ (d) $^{90}_{229}X$ (e) $^{228}_{90}X$ (f) $^{230}_{100}X$ (g) $^{229}_{90}X$

2.41 Select the isotopes from the list below: (a) $^{233}_{92}X$ (b) $^{92}_{234}X$ (c) $^{234}_{92}X$ (d) $^{232}_{92}X$ (e) $^{92}_{233}X$ (f) $^{100}_{40}X$

2.42 Fill the table below indicating the number of electrons (n_e), neutrons (n_n) and protons (n_p) for the follow-

ing neutral atoms:

	Isotope	n_e	n_p	n_n
a	$^{14}_7\text{N}$			
b	$^{15}_7\text{N}$			
c	$^{13}_7\text{N}$			

2.43 Fill the table below indicating the number of electrons (n_e), neutrons (n_n) and protons (n_p) for the following neutral atoms:

	Isotope	n_e	n_p	n_n
a	$^{134}_{55}\text{Cs}$			
b	$^{135}_{55}\text{Cs}$			
c	$^{137}_{55}\text{Cs}$			

2.44 Fill the table below indicating the number of electrons (n_e), neutrons (n_n) and protons (n_p) for the following charged atoms:

	Isotope	n_e	n_p	n_n
a	$^{48}_{20}\text{Ca}^{+2}$			
b	$^{18}_{9}\text{F}^{-}$			
c	$^{62}_{28}\text{Ni}^{3+}$			

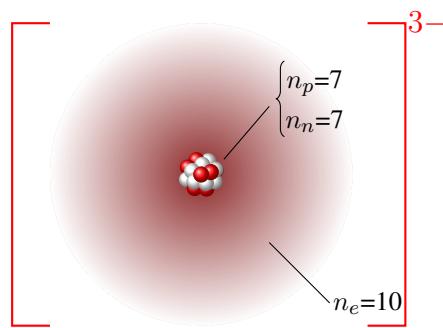
2.45 Fill the table below indicating the number of electrons (n_e), neutrons (n_n) and protons (n_p) for the following charged atoms:

	Isotope	n_e	n_p	n_n
a	$^{147}_{61}\text{Pm}^{+}$			
b	$^{192}_{77}\text{Ir}^{-}$			
c	$^{209}_{83}\text{Bi}^{-2}$			

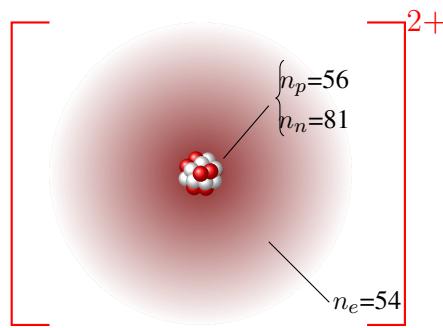
2.46 Calculate the number of protons, neutrons and electrons in the following isotopes: (a) $^{15}_7\text{N}$ (b) $^{64}_{29}\text{Cu}$ (c) $^{93}_{40}\text{Zr}$

2.47 Calculate the number of protons, neutrons and electrons in the following isotopes: (a) $^{79}_{34}\text{Se}$ (b) $^{85}_{36}\text{Kr}$ (c) ^{13}N

2.48 Write down the isotopic symbol for the atom or ion represented below indicating the name of the element.



2.49 Write down the isotopic symbol for the atom or ion represented below indicating the name of the element.



2.50 Write down the isotopic symbol given the number of protons, neutrons and electrons: (a) 43 protons, 43 electrons and 60 neutrons (b) 48 protons, 48 electrons and 65 neutrons (c) 77 protons, 77 electrons and 115 neutrons

2.51 Write down the isotopic symbol given the number of protons, neutrons and electrons: (a) 93 protons, 93 electrons and 142 neutrons (b) 55 protons, 55 electrons and 79 neutrons (c) 52 protons, 52 electrons and 72 neutrons

2.52 The atomic mass of Ga is 69.72 amu. There are only two naturally occurring isotopes of gallium: ^{69}Ga , with a mass of 69.0 amu, and ^{71}Ga , with a mass of 71.0 amu. Calculate the natural abundance of the ^{69}Ga isotope.

2.53 The atomic mass of Xe is 131.293 amu. There are only two naturally occurring isotopes of Xe: Xenon-133, with a mass of 133.0 amu, and Xenon-135, with a mass of 135 amu. Calculate the natural abundance of the Xenon-135 isotope.



2.54 Magnesium contains three different isotopes: magnesium-24 with an abundance of 79% and a mass of 23.9850423 amu, magnesium-25 with an abundance of 10% and a mass of 24.9858374 amu, and magnesium-26 with a mass of 25.9825937 amu. Calculate the abundance of magnesium-26 and the average atomic mass of a sample of magnesium.

2.55 Silicon contains three different isotopes: Si-28 with a mass 27.976927 amu and abundance of 92.2297%, Si-29 with a mass 28.976495 amu and abundance of 4.6832% and Si-30 with a mass 29.973770 amu. Calculate the abundance of Si-30 and the average atomic mass of a sample of Si.

2.56 There are only two naturally occurring isotopes of Lutetium: Lu-175 with a mass of 174.94 amu and abundance of 97.41%, and Lu-176 with a mass of 175.94 amu and abundance of 2.59%. Calculate the average mass of the element using the table below, given m_i is the isotopic mass and f_i is the fractional abundance of the isotope.

Isotope	m_i , amu	f_i	$m_i \times f_i$
<hr/>			
Average mass =		$\sum m_i \times f_i =$	
amu			

2.57 There are only two naturally occurring isotopes of Thallium: Tl-203 with mass of 202.972 amu and abundance of 29.52%, and Tl-205 with mass of 204.974 amu and abundance of 70.48%. Calculate the average mass of the element using the table below, given m_i is the isotopic mass and f_i is the fractional abundance of the isotope.

Isotope	m_i (amu)	f_i	$m_i \times f_i$
<hr/>			
Average atomic mass (amu)		$\sum m_i \times f_i =$	

2.58 Fill the table below and calculate the missing variable.

Isotope	m_i (amu)	f_i	$m_i \times f_i$
^{107}Ag	106.9050	0.5184	?
^{109}Ag	108.9047	0.4816	?
Average atomic mass			$= \sum m_i \times f_i = ?$
			(amu)

2.59 Fill the table below and calculate the missing variable.

Isotope	m_i (amu)	f_i	$m_i \times f_i$
^{137}Ba	136.9058	?	?
^{138}Ba	137.9052	?	?
Average atomic mass			$= \sum m_i \times f_i = 114.38$
			(amu)

AN INTRODUCTION TO MOLECULES

2.60 Calculate the molecular mass of the following compound: CCl_2F_2

2.61 Calculate the molecular mass of the following compound: C_4H_{10}

2.62 Calculate the molecular mass of the following compound: $\text{C}_6\text{H}_{10}\text{O}_8$

2.63 Calculate the molecular mass of the following compound: C_6H_6

EMPIRICAL AND MOLECULAR FORMULAS

2.64 What is the empirical formula of a compound if a sample of this compound contains 2.8 g of nitrogen and 3.2 g of oxygen?

2.65 What is the empirical formula and the molecular formula of a compound if a sample contains 3 g of C, 0.5 H and 4 g of oxygen? MW=60 amu



2.66 What is the empirical and molecular formula of a compound with a percent composition of 49.47% C, 5.201% H, 28.84% N, and 16.48% O, if its molecular mass is 194.2 amu.

2.67 A 1.587 g sample of a compound containing N and O was analyzed finding a composition of 0.483 g of Nitrogen and 1.104 g of Oxygen. Calculate the empirical formula of the compound.

Ch. 3. Chemical naming

ALL elements in the periodic table except for the noble gases—He, Ne, Ar, Kr, Xe, and Rn—combine to produce chemical compounds. Most of these chemicals are useful in your everyday life, and you drink water to quench your thirst, use Clorox to clean your house, or baking soda to get rid of a stinky refrigerator. In this chapter you will learn not only how to name these chemicals but also read chemical formulas—we call this to formulate chemicals. Still, chemical elements such as hydrogen and oxygen do not combine randomly and they only choose specific elemental partners to form a compound. As an example, hydrogen combines with oxygen using specific proportions to produce H_2O and not HO_2 . In this chapter, you will also learn the rules that chemical elements use to combine.

3.1 Ions & ionic charges

Atoms gain and lose electrons to produce ions. An ion is just an atom with a positive or negative charge. Ions result from an electron transfer. Positive ions have lost negatively charged electrons, whereas negative ions have gained electrons. The reason for this electron transfer is that atoms try to achieve a very stable electronic configuration with eight electrons in the valence, and this is called the octet electron configuration. Examples of ions are: H^+ , Ca^{2+} or O^{2-} . This section covers the properties of ions and ionic charges.

Cations and anions Atoms that lose electrons become positively charged. These ions are called cations. Examples of cations are Li^+ or Mg^{2+} called lithium cation and magnesium cation, respectively. Atoms that gain electrons become negatively charged, as electrons have a negative charge. These ions are called anions. Examples of anions are F^- called fluoride or N^{3-} called nitride. The way to name anions is by using the name of the element and the suffix -ide.

The figure shows a periodic table where each element's common ionic charge is indicated in its respective square. A legend at the top identifies three types of charges: Anions (blue), Cations (red), and Transition metal Cations (orange). The table includes the following data:

- Anions:** F⁻, O²⁻, N³⁻, S²⁻, Cl⁻, Br⁻, I⁻.
- Cations:** H⁺, Li⁺, Be²⁺, Na⁺, Mg²⁺, K⁺, Ca²⁺, Rb⁺, Sr²⁺, Cs⁺, Ba²⁺, Ag⁺, Cd²⁺, Cu⁺, Cu²⁺, Zn²⁺, Ga³⁺, Sn²⁺, Sn⁴⁺, Pb²⁺, Pb⁴⁺.
- Transition metal Cations:** Cr²⁺, Cr³⁺, Mn²⁺, Mn³⁺, Fe²⁺, Fe³⁺, Co²⁺, Co³⁺.

Figure 3.1 Ionic charges (valences) for different elements

Ionic charges: the valences How do we know that hydrogen produces a



H^+ ion and nitrogen a N^{3-} anion? The charge of an ion is called an ionic charge, and the numbers are coming from the periodic table. H, Na, or K are in group IA (left of the table) and hence the ionic charge will be $1+$. Similarly, Mg or Ca are in group IIA (left of the table) and hence the ionic charge will be $2+$. Differently, F, Cl, or Br are in group 7A (right of the table) and their charge will be $1-$. Oxygen is in group 6A (right of the table) and the ionic charge will be $2-$. Figure ?? contains all ionic charges. What if the element is not on this list such as in the case of Iron (Fe)? In that case, very probably it will have several ionic charges and this charge has to be indicated in the chemical name. An example would be Fe, which ionic charge is not in Figure ?? as iron can have several ionic charges.

Sample Problem 24

Identify the correct ionic state of the following elements: (a) Cl (b) K (c) O
(d) C

SOLUTION

Cl is on the 7A group and hence its charge is $1-$, whereas potassium belongs to 1A and its charge will be $1+$. Oxygen and carbon will have $2-$ and $4-$ charges. The final ionic states are: Cl^- , K^+ , O^{2-} and C^{4-} .

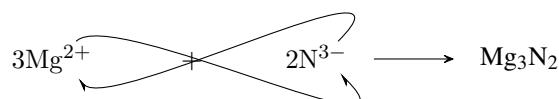
❖ STUDY CHECK

Identify the correct ionic state of the following elements: (a) N (b) Br

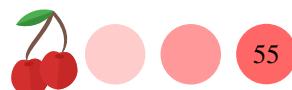
3.2 Ionic compounds

Ionic compounds are chemicals resulting from the combination of a nonmetallic element with a metallic element. An example is NaCl , which results from combining sodium (a metal) with chloride (a nonmetal). Ionic compounds normally have high melting points and are solid under normal conditions. A typical ionic compound would be NaCl , cooking salt. Atoms of an ionic compound are connected through an ionic bond. In an ionic bond, one element gives away electrons (the cation) and the other one receives electrons (the anion). As an example, in the NaCl molecule Na gives away an electron to Cl, and the molecule results from the combinations of Na^+ and Cl^- . In an ionic compound, the element on the left is positive and the one on the right is negative.

Combining ions Ionic compounds are the result of combining two ions: a positive (cation) and a negative (anion) ion. Each ion has a charge, depending on its location on the table. When combining two atoms you first need to arrange the ions starting from positive and followed by negative. The charges of an ion would become the coefficient of the other ion. For example Mg^{2+} and N^{3-} are combined as Mg_3N_2 :



Another example would be the combination of Na^+ and O^{2-} that would be Na_2O . You need to simplify the indexes of the formula by dividing by the smallest one, always using integer values. For example, Mg^{2+} and O^{2-} give Mg_2O_2 that should be written as MgO



Another example that involves simplifying the formula is the chemical result of combining Ca^{2+} and C^{4-} . After combining the charges we obtain Ca_4C_2 that needs to be simplified by dividing by the smallest number leading to Ca_2C .

Sample Problem 25

Combine the following ions or give the ions given the final compound: (a) Li^+ and O^{2-} (b) Ca^{2+} and O^{2-} (c) Li_3N (d) Mg_2C

SOLUTION

The result of combining Li^+ and O^{2-} is Li_2O . For Ca^{2+} and O^{2-} , the resulting chemical is CaO . Li_3N results from the combination of Li^+ and N^{3-} , and Mg_2C results from Mg^{2+} and C^{4-} .

◆ STUDY CHECK

Combine the following ions or give the ions given the final compound: (a) Na^+ and F^- (b) Na_3N

Simple ionic naming (type I ionic) Type I ionic compounds result from the combination of a metal with given valence (Li, Ca, Mg, etc, see Figure 3.1) and a nonmetal. To name an ionic compound (type I ionic) you need to (a) use the name of the first element in the compound, (b) use the first syllable of the second element, and (c) finish the name of the molecule in the suffix *-ide*. As an example, the formula NaCl is named sodium chloride, and MgCl_2 is named magnesium chloride. Another example would be:

calcium chloride

CaCl_2 (ionic)

To formulate an ionic compound based on a name, we need to combine both ions by exchanging the valences (the ionic charges). For example, MgCl_2 results from the combination of Mg^{2+} and Cl^- so that the number 2 in MgCl_2 near the Cl atom is coming from the Mg^{2+} . In other words:



The sign of the charges only indicates which element goes first in the formula: the positive element (cation) first followed by the negative element (anion). For example, the result of combining Na^+ and Cl^- is NaCl and not ClNa as Na has a positive ionic charge and has to appear first in the formula.

Sample Problem 26

Name or give the formula for the following ionic compounds: (a) MgO (b) Mg_3N_2 (c) Lithium nitride (d) Magnesium carbide

SOLUTION

The name for MgO is magnesium oxide. Mg_3N_2 is called magnesium nitride. The formula for Lithium nitride is Li_3N and the formula for Magnesium carbide is Mg_2C , result of simplifying Mg_4C_2 dividing by two, the smallest number.



❖ STUDY CHECK

Name or give the formula for the following ionic compounds: (a) Sodium fluoride (b) Na_3N

The ionic chemical NaCl results from the combination of Na^+ and Cl^- . The ionic charges of Na and Cl are given in Figure ?? according to the group. If the ionic chemical contains a transition metal with variable ionic charge, that is, which is not in Figure ?? then the ionic naming becomes a bit more complex. The reason is that one needs to specify the charge of the metal, explicitly in the name of the chemical. An example would be NiCl_2 named as Nickel(II) chloride or Co_2O_3 named as Cobalt(III) oxide.

Name complex ionic chemicals This section covers how to name ionic chemicals containing a metal with variable charge. In this case, you need to specify the charge of the metal in the name. To calculate this number you will solve a simple math equation. For example, the name of Mn_2O_3 is Manganese(III) oxide. How do we get this name? Manganese has several charges as it is not in Figure ??, let us use x for its charge Mn^x and oxygen has a charge of two O^{2-} . After combining Mn^x and O^{2-} the resulting formula would be Mn_2O_x . By comparison with the given formula, Mn_2O_3 , x has to be three and hence the charge of Mn has to be three. Therefore, the final name would be Manganese(III) oxide.

Properties of ionic compounds Ionic compounds normally have high melting points and are solid under normal conditions. A typical ionic compound would be NaCl , cooking salt.

The ionic bond Atoms of an ionic compound are connected through an ionic bond. In an ionic bond, one element gives away electrons (the cation) and the other one receives electrons (the anion). As an example, in the NaCl molecule Na gives away an electron to Cl, and the molecule results from the combinations of Na^+ and Cl^- . In an ionic compound, the element on the left is positive and the one on the right is negative.

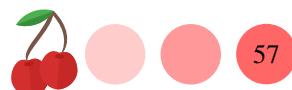
Sample Problem 27

Name or give the formula for the following ionic compounds: (a) MnO (b) Fe_3N_2 (c) Cobalt(II) carbide (d) Iron(II) oxide

SOLUTION

All the chemicals on this example contain a metal that can have several charges, and hence, we need to specify the ionic charge on the name. MnO results from Mn^x and O^{2-} . After combining the ions, the formula would be Mn_2O_x , a formula that needs to be compared to MnO . The formulas do not look similar, so lets make them more similar by dividing by two so that $\text{MnO}_{\frac{x}{2}}$ resembles MnO . By comparing x has to be 2 and hence the name is Manganese(II) oxide. The name for Fe_3N_2 would be Iron(II) nitride. The valence of Iron comes from combining Fe^x and N^{3-} that gives Fe_3Nx . By comparison with Fe_3N_2 x has to be two and the name is Iron(II) nitride. the formula for Cobalt(II) carbide would be Co_2C as Cobalt(II) is Co^{2+} and carbide is C^{4-} . After combining the ions one obtains Co_4C_2 that gives Co_2C . Finally, the formula for Iron(II) oxide is FeO as Iron(II) is Fe^{2+} and oxide is O^{2-} that gives Fe_2O_2 and simplifying one obtains FeO .

❖ STUDY CHECK



Name or give the formula for the following ionic compounds: (a) Manganese(IV) oxide (b) AuCl_3

3.3 Covalent compounds

Covalent compounds are chemicals resulting from the combination of nonmetallic elements. An example is CO_2 , which results from combining carbon (a nonmetal) with oxygen (a nonmetal). At normal conditions, covalent compounds may exist as solids, liquids, or gases. Covalent compounds do not exhibit any electrical conductivity, either in pure form or when dissolved in water. A typical covalent compound would be H_2O , water. Atoms in a covalent compound are connected by means of a covalent chemical bond. In a covalent bond, both atoms connected share the electrons. As an example, the HCl molecule has an hydrogen and a chlorine atom connected by means of a covalent bond, in which each atoms share the electrons of the bond.

Covalent naming To name a covalent compound you need to (a) use the name of the first element in the compound, (b) use the first syllable of the second element, and (c) finish the name of the molecule in the suffix *-ide*. More importantly, you need to use prefixes (see Table ??) that indicate the number of atoms in the molecule. See the Table below for a list of the different equivalencies between prefixes and numbers. As an example, the formula CH_4 is named carbon tetrahydride. Similarly, a covalent chemical name can be translated into a formula (we call this to formulate a chemical with a given name), and the formula for carbon monoxide would be CO . When the vowels *a* and *o* appear together, the first vowel is omitted as in carbon monoxide instead of carbon ~~monooxide~~. Another example would be N_2O named as dinitrogen oxide, and the name sulfur hexafluoride corresponds to the formula SF_6 . The prefix mono is omitted in the first element of the name, and for example, you will not name the chemical CO as ~~monoearbon~~ monoxide, you would just say carbon monoxide. A final example of a covalent compound:

dinitrogen pentoxide

N_2O_5 (covalent)

Table 3.3 Prefixes used to name covalent compounds

Prefix	number	Prefix	number	Prefix	number
Mono	1	Tetra	4	Hepta	7
Di	2	Penta	5	Octa	8
Tri	3	Hexa	6	Nona	9

Sample Problem 28

Name or give the formula for the following covalent chemicals: (a) NO (b) CS_2 (c) Sulfur Dioxide (d) Nitrogen Trichloride

SOLUTION

All chemicals in this example are covalent as they result of the combination of nonmetals. In order to name them, we need to use prefixes and finish the suffix



with -ide. The first chemical is called nitrogen monoxide. CS_2 is called carbon disulfide. The formula for sulfur dioxide and nitrogen trichloride are respectively SO_2 and NCl_3 .

STUDY CHECK

Name or give the name of the following covalent chemicals: (a) SCl_2 (b) diboron trioxide

3.4 Naming acids & bases

In this section, we will learn how to name acids and bases. Acids normally have common names (e.g. sulfuric acid) and their naming does not follow modern rules. Names and formulas of acids are listed in tables. Differently, bases (e.g. sodium hydroxide) are named in a standard way.

Bases or hydroxides Bases (hydroxides) result from the combination of metal and the hydroxide anion (OH^-). Examples are NaOH or $\text{Ca}(\text{OH})_2$. The name of a base starts with the name of the cation finishing with the word *hydroxide*. An example is NaOH named as *sodium hydroxide*, or $\text{Ca}(\text{OH})_2$, named as *calcium hydroxide*. The word *hydroxide* refers to the OH^- ion, and hence Sodium hydroxide results from combining Na^+ and OH^- , and Calcium hydroxide from combining Ca^{2+} and OH^- . More examples of hydroxides:

Magnesium hydroxide

$\text{Mg}(\text{OH})_2$ (hydroxide)

As a final note, not all bases are hydroxides. For example, ammonia NH_3 is a base even when it does not contain hydroxides in its structure. A way to remember this is sometimes to write ammonia like NH_4OH .

Acids Acids—in particular inorganic acids—are chemicals that normally contain hydrogen at the beginning of their formula. For example, HCl or H_2SO_4 . HCl is a hydracid and is named as *hydrochloric acid*, whereas H_2SO_4 is an oxoacid that contains oxygen named as *sulfuric acid*. The names of acids are not standard and they come from common names employed in the field for many years. Table ?? contains a list of the most important oxoacids and hydracids. More examples of acids:

Nitric acid

HNO_3 (oxoacid)

Hydrofluoric acid

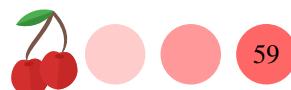
HF (hydracid)

Sample Problem 29

Name or give the formula for the following acids and bases. Indicate whether the compound is an acid or a base. (a) HCN (b) KOH (c) Carbonic acid (d) Lithium hydroxide

SOLUTION

HCN is an acid named hydrocyanic acid. KOH is a base called potassium hydroxide. The formula for Carbonic acid is H_2CO_3 , and Lithium hydroxide is



a base with formula LiOH.

STUDY CHECK

Name or give the formula for the following ionic compounds: (a) phosphoric acid (b) Mg(OH)₂

3.5 Oxidation states

Isolated atoms tend to have a neutral state. However, the atoms of elements have the capacity of gaining and losing electrons forming cations and anions. The atoms that form a compound can have different states resulting in losing and gaining electronic charge. We refer to this as the oxidation state of an element in a compound.

Oxidation states of oxoacids Consider the following set of acids: HClO, HClO₂, HClO₃ and HClO₄. We say Cl in these acids have different oxidation states or different oxidation numbers. This section will cover the calculation of the oxidation state of the central atom of an oxoacid.

Let us address the oxoacid: HClO₃. The goal is to calculate the oxidation number of the underlined element, Cl. To do this we will follow a set of simple rules. First, we will use the valences as the oxidation number of the elements (see Figure 3.1) to the right and the left of the central atom. Then, we will assign an unknown oxidation state of x to the central atom. After that, we will set up an equation so that the sum of all oxidation numbers equals the charge of the acid if any. In this formula, we will include the atomic coefficients. In the case of HClO₃, the equation would be:

$$1 + x + 3 \cdot (-2) = 0$$

as the number of oxygens is three, we will have to time by three the valence of oxygen. The number zero results from the charge of the acid. If we solve for x , we obtain $x = 5$. That is, the oxidation state of Cl on HClO₃ is 5 and this is represented as HCl^VO₃.

Oxidizing and reducing character of oxoacids The importance of the oxidation state of the central elements of oxoacid results from the fact that acids with high or low oxidation states, tend to be very reactive, sometimes capable of completely dissolving metals. We call this oxidizing (or reducing) acids. For example, HNO₃ and H₂SO₄ are both oxidizing acids, and these acids will dissolve for example a piece of copper. Similarly, acids with very small or negative oxidation numbers can be very reactive as well. These acids are called reducing acids or agents. Let us compare two oxoacids to elaborate more on the terminology used to describe redox numbers. For example, let us compare HCl^VO₃ and HCl^{III}O₂. We say Cl on HCl^VO₃ has a larger redox number than HCl^{III}O₂. We can also say, Cl in HCl^VO₃ is more oxidized than Cl on HCl^{III}O₂. Finally, we can also say, HCl^VO₃ is more reducing than HCl^{III}O₂. Again, the terms associated with high redox numbers are oxidized and reducing, and the terms associated with low redox numbers are reduced and oxidizing.

It is important to note that ultimately the oxidation state of an element is related to the number of electrons of the element. The more electrons the smaller—the more negative—the oxidation state. In other words, large oxidation states result from losing electrons.



Sample Problem 30

Calculate the redox number of S in the following acids and indicate the more oxidizing acid: $\text{H}_2\text{S}_2\text{O}_6$ named dithionic acid and H_2SO_4 named sulfuric acid.

SOLUTION

We will set up the redox formula for the first acid ($\text{H}_2\text{S}_2\text{O}_6$), given that the redox number of H is +1 and the redox number of O is -2.

$$2 \cdot 1 + 2 \cdot x + 6 \cdot (-2) = 0$$

Solving for x:

$$2 + 2 \cdot x - 12 = 0 \quad \text{we have that } x = \frac{12 - 2}{2}$$

The oxidation state of S in $\text{H}_2\text{S}_2\text{O}_3$ is +5. For the second acid (H_2SO_4):

$$2 \cdot 1 + x + 4 \cdot (-2) = 0$$

Solving for x:

$$2 + x - 8 = 0 \quad \text{we have that } x = \frac{8 - 2}{1}$$

that gives a redox of 6. If we compare both acids the smaller the redox number the more reduced is the central element and the more oxidizing the acid is. Therefore, $\text{H}_2\text{S}_2\text{O}_3$ is more oxidizing than H_2SO_4 .

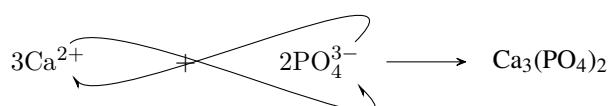
◆ STUDY CHECK

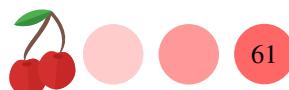
Calculate the redox number of the following acids: (a) H_2MnO_4 (b) $\text{H}_2\text{Cr}_2\text{O}_7$

3.6 Naming complex salts & common chemicals

At this point, we saw the naming and formulation of ionic (e.g. NaCl) and covalent compounds (e.g. CO_2). This section covers the naming of complex salts: oxosalts and hydrosalts. In general, salts (oxosalts or hydrosalts) are the result of mixing an oxoacid and a base. They tend to look more complex than simple ionic or covalent compounds as they have at least three different elements. An example of oxosalt would be CaSO_4 called calcium carbonate. An example of hydrosalt would be NaHSO_4 which is called sodium monohydrosulfate. This section will also cover the naming of hydrates (e.g. $\text{CaSO}_4 \cdot \text{H}_2\text{O}$), which are compounds containing water molecules inside their structure. Before being able to name these complex chemicals it is convenient to practice combining ions, without paying attention to the naming.

Combining ions To combine two ions, you first arrange the positive ion on the left followed by the negative ion on the right, to then cross the ionic charges from the top of the ion to the bottom of the opposite ion. The positive and negative charges are not carried. If the ions have more than one element we have to use parenthesis. An example would be combining Ca^{2+} and PO_4^{3-} leading to $\text{Ca}_3(\text{PO}_4)_2$:





We would simplify in case the charges compensate for each other.

An example would be combining Mg^{2+} and SO_4^{2-} leading to $MgSO_4$



Table 3.2 Names of oxoacids and oxosalts (top table) and hyracids (bottom table).*

Element	Oxoacid	Oxoacid Name	Oxoasalt	Oxoasalt Name
Manganese	$HMnO_4$	Permanganic Acid	MnO_4^-	Permanganate
	H_2MnO_4	Manganic acid	MnO_4^{-2}	Manganate
Carbon	H_2CO_3	Carbonic Acid	CO_3^{-2}	Carbonate
Nitrogen	HNO_3	Nitric Acid	NO_3^-	Nitrate
	HNO_2	Nitrous Acid	NO_2^-	Nitrite
Phosphorus	H_3PO_4	Phosphoric Acid	PO_4^{-3}	Phosphate
Sulfur	H_2SO_4	Sulfuric Acid	SO_4^{-2}	Sulfate
	H_2SO_3	Sulfurous Acid	SO_3^{-2}	Sulfite
	$H_2S_2O_2$	Thiosulfurous Acid	$S_2O_2^{-2}$	Thiosulfite
	$H_2S_2O_3$	Thiosulfuric Acid	$S_2O_3^{-2}$	Thiosulfate
	$H_2S_2O_7$	Disulfuric acid	$S_2O_7^{-2}$	Disulfate
	$H_2S_2O_8$	Peroxodisulfuric acid	$S_2O_8^{-2}$	Peroxodisulfate
Chlorine	$HClO_4$	Perchloric Acid	ClO_4^-	Perchlorate
	$HClO_3$	Chloric acid	ClO_3^-	Chlorate
	$HClO_2$	Chlorous acid	ClO_2^-	Chlorite
	$HClO$	Hypochlorous acid	ClO^-	Hypochlorite
Iodine	HIO_4	Periodic Acid	IO_4^-	Periodate
Chromium	H_2CrO_4	Chromic acid	CrO_4^{2-}	Chromate
	$H_2Cr_2O_7$	Dichromic acid	$Cr_2O_7^{2-}$	Dichromate
Boron	H_3BO_3	Boric acid	BO_3^{3-}	Borate
Hydracid	Hydracid Name	Hydracid	Hydracid Name	
HCl	Hydrochloric acid	HBr	Hydrobromic acid	
HI	Hydroiodic acid	HF	Hydrofluoric acid	
HCN	Hydrocyanic acid	H_2S	Hydrosulfuric acid	

* Yellow indicate very important acids

Naming Oxosalts The names of the oxosalts are constructed by combining the name of the first element—you need to specify its charge in the case of a transition metal element with different possible charges—followed by the name of the oxosalt from Table ???. For example, the name of $MgSO_4$ is magnesium sulfate, as Mg^{2+} is magnesium and SO_4^{2-} is sulfate. Another example is $Fe_2(CO_3)_3$ called Iron(III) carbonate. A final example:

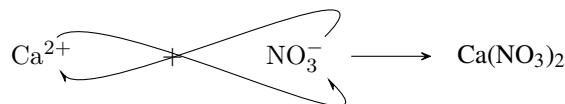
Lithium nitrate

$LiNO_3$ (oxosalt)

Formulating Oxosalts In the case that you know the name of an oxosalt and you want to obtain its formula, you first need to arrange the positive ion on the left followed



by the negative ion on the right, to then cross the ionic charges from the top of the ion to the bottom of the opposite ion. For example, calcium nitrate results from the combination of Ca^{2+} calcium and NO_3^- , nitrate. By combining the two ions we obtain the final formula as $\text{Ca}(\text{NO}_3)_2$:



Sample Problem 31

Name of give the name of the following oxosalts: (a) K_2SO_4 (b) Na_2CO_3
(c) Magnesium carbonate (d) Sodium phosphate

SOLUTION

K_2SO_4 is named potassium sulfate, as K^+ is potassium and SO_4^{2-} stands for sulfate. Na_2CO_3 is sodium carbonate. Magnesium carbonate is MgCO_3 and sodium phosphate is Na_3PO_4 .

◆ STUDY CHECK

Name of give the name of the following oxosalts: (a) CaSO_4 (b) Aluminum sulfate

Some oxosalts contain hydrogen atoms in their structure between the oxosalt cation and anion (e.g. NaHSO_4). For example, NaHSO_4 is named sodium monohydrogen-sulfate. To understand this name, we will first focus on the second part of the name, monohydrogensulfate which represents the anion. The name monohydrogensulfate (HSO_4^-) comes from adding a proton (H^+) to a sulfate cation (SO_4^{2-}). Mind that protons (H^+) are positively charged and therefore if we add a single H^+ to a sulfate cation (SO_4^{2-}) the charge will have to decrease a single unit, giving us HSO_4^- . As we can see, the name is directly related to the oxosalt anion and the number of hydrogens in the hydrosalt name. For example, phosphate (PO_4^{3-}) is an oxosalt anion whereas hydrogenphosphate (HPO_4^{2-}) and dihydrogenphosphate (H_2PO_4^-) are both hydrosalt anions. An explanation about the charges: as phosphate has three negative charges, hydrogenphosphate has to have one less charge (that is $2-$) and dihydrogenphosphate has to have two less negative charges (that is -1). Some final hydrosalt anions examples:

carbonate

CO_3^{-2} (oxosalt ion)

monohydrogen carbonate

HCO_3^- (hydrosalt ion)

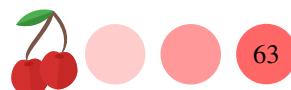
Above we saw how to name just the ending of the oxosalt with hydrogen anion. Now we can move forward to the whole naming of the salt. We just need to add the name of the element in the first place, and for example, NaH_2BO_3 would be named sodium dihydrogenborate. If the first ion—the cation—is a transition metal cation (a type two cation) we need to include in parenthesis the valence of the cation. For example, $\text{Fe}(\text{H}_2\text{BO}_3)_2$ would be named iron(II) dihydrogenborate. More examples:

sodium carbonate

Na_2CO_3 (oxosalt)

sodium monohydrogen carbonate

NaHCO_3 (hydrosalt)

**Sample Problem 32**

Name or formulate the following hydrosalts: (a) Magnesium hydrogensulfate
(b) Sodium hydrogen carbonate (c) LiHCO₃ (d) Mg(H₂PO₄)₂

SOLUTION

The formula of Magnesium hydrogensulfate is Mg(HSO₄)₂ as the formula for monohydrogen sulfate is HSO₄⁻ and the valence of magnesium is Mg²⁺. The formula for Sodium monohydrogen carbonate is NaHCO₃ as it results from combining Na⁺ and HCO₃⁻. Mind monohydrogen carbonate results from adding a hydrogen ion H⁺ to a carbonate CO₃²⁻ ion. The name for LiHCO₃ is lithium monohydrogen carbonate, whereas the name for Mg(H₂PO₄)₂ is magnesium dihydrogenphosphate.

◆ STUDY CHECK

Name or formulate the following hydrosalts: (a) LiHS₂O₃ (b) LiH₂PO₄
(c) sodium hydrogenphosphate

Naming oxosalts with hydrates Some chemicals contain water molecules trapped in their structure and therefore water molecules (H₂O) are often indicated in chemical formulas. These types of chemicals containing water are called *hydrates*, precisely because hydrate means water. Examples of hydrates are BeSO₄ · 4 H₂O or CuSO₄ · 5 H₂O called respectively beryllium sulfate tetrahydrate and copper(II) sulfate pentahydrate. To formulate hydrates you just need to use prefixes such as mono, di, tetra—the same ones we use to name covalent chemicals, see Table ??—to indicate the number of water molecules in the chemical and end the name with *hydrate*. As a note, warming up hydrates (e.g. BeSO₄ · 4 H₂O) results in the release of water producing a dehydrated or *anhydrous* compound (e.g. BeSO₄). A final example of hydrate naming:

Sodium sulfate pentahydrate

Na₂SO₄ · 5 H₂O (a hydrate)**Sample Problem 33**

Name or formulate the following hydrates: (a) Nickel(II) permanganate dihydrate
(b) Sodium nitrate monohydrate (c) Na₂CO₃ · 10 H₂O (d) MgSO₄ · 7 H₂O

SOLUTION

The formula for Nickel(II) permanganate is Ni(MnO₄)₂, therefore the formula for Nickel(II) permanganate dihydrate is Ni(MnO₄)₂ · 2 H₂O. The formula for Sodium nitrate is NaNO₃, therefore NaNO₃ · H₂O is Sodium nitrate monohydrate. The name for Na₂CO₃ · 10 H₂O is sodium carbonate decahydrate and MgSO₄ · 7 H₂O is magnesium sulfate heptahydrate.

◆ STUDY CHECK

Name or formulate the following hydrates: (a) LiNO₃ · H₂O (b) Na₃PO₄ · 3 H₂O
(c) sodium sulfate tetrahydrate

Common naming Some of the chemicals are normally referred to by a common name that does not involve the use of any chemical naming rules. An example would be H₂O normally referred to as water instead of its standard name which is dihydrogen oxide. You can find more names in Table 3.3. Another example:



NaCl

Sodium chloride (standard name)

Table salt (common name)

Table 3.3 List of common chemicals

Chemical	Name	Chemical	Name
H ₂ O	Water	Mg(OH) ₂	Milk of magnesia
NH ₃	Ammonia	N ₂ O	Laughing gas
CH ₄	Methane	CaCO ₃	Marble
CO ₂	Dry ice	CaO	Quicklime
NaCl	Table salt	NaHCO ₃	Baking Soda
NaHCO ₃	Sodium Bicarbonate	MgSO ₄ · 7 H ₂ O	Epsom Salt

Sample Problem 34

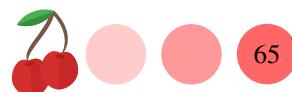
Name or formulate the following common chemicals: milk of magnesia and dry ice.

SOLUTION

The formula for milk of magnesia is Mg(OH)₂ (magnesium hydroxide), whereas dry ice is the common name for CO₂, carbon dioxide.

❖ STUDY CHECK

Name or formulate the following common chemicals: (a) ammonia (b) methane



CHAPTER 3

IONS & IONIC CHARGES

3.1 Indicate if the following chemical species represent an atom, and anion or a cation: (a) Fe^{2+} (b) Cl^- (c) Ag

3.2 Indicate if the following chemical species represent an atom, and anion or a cation: (a) Cs (b) Cs^+ (c) N^{-3}

3.3 Identify the ionic state of the following elements. If needed, indicate the existence of multiple ionic states:
(a) H (b) O (c) N (d) F (e) Mn

3.4 Identify the ionic state of the following elements. If needed, indicate the existence of multiple ionic states:
(a) Li (b) V (c) Cl (d) S (e) Cr (f) Sr (g) Ni

COVALENT COMPOUNDS

3.5 Name or formulate the following covalent compounds: (a) NO (b) Dichlorine monofluoride (c) NO_2

3.6 Name or formulate the following covalent compounds: (a) Chlorine Monofluoride (b) N_2O (c) Nitrogen trifluoride

3.7 Name or formulate the following covalent compounds: (a) SO_3 (b) Disulfur dichloride (c) SO_2 (d) Disulfur tetrachloride

3.8 Name or formulate the following covalent compounds: (a) P_4S_3 (b) Sulfur Tetrafluoride (c) As_2O_5 (d) Sulfur trioxide

IONIC COMPOUNDS

3.9 Classify the following chemicals in two groups, justifying your classification: (a) NaCl (b) CO_2 (c) FeCl_3 (d) N_2O_3 (e) SO_3 (f) Ca_3N_2

3.10 Combine the following ions:

- | | |
|--------------------------------------|--|
| (a) Na^+ + Cl^- | (d) Mg^{2+} + Cl^- |
| (b) Na^+ + Se^{2-} | (e) Mg^{2+} + O^{2-} |
| (c) Na^+ + P^{3-} | (f) Mg^{2+} + N^{3-} |

3.11 Name or formulate the following ionic (Type I) compounds: (a) Magnesium iodide (b) Ca_3P_2 (c) Lithium nitride (d) MgF

3.12 Name or formulate the following ionic (Type I) compounds: (a) Magnesium fluoride (b) CaS (c) Barium phosphide (d) Mg_3N_2

3.13 Name the following compounds:

- | | |
|-----------------------------|-------------------|
| (a) NaCl | (d) SrS |
| (b) Ca_3N_2 | (e) RbCl |
| (c) MgI_2 | (f) KF |

3.14 Combine the following ions:

- | | |
|--|--|
| (a) Cs^+ + F^- | (c) Be^{2+} + C^{4-} |
| (b) Sr^{2+} + O^{2-} | (d) Li^+ + I^- |

3.15 Classify the following chemicals in two groups. Justify your classification.

- | | | |
|--------------------|---------------------|---------------------------|
| (a) NaCl | (c) FeCl_3 | (e) Li_3N |
| (b) MnO_2 | (d) SrO | (f) NiO |

3.16 Formulate the following compounds:

- | | |
|------------------------|-------------------------|
| (a) Copper(I) oxide | (c) Nickel(III) oxide |
| (b) Copper(II) nitride | (d) Manganese(IV) oxide |

3.17 Name the following compounds:

- | | |
|-----------------------------|--------------------|
| (a) NiO | (c) VO |
| (b) Cr_2O_3 | (d) MnO_4 |

3.18 Formulate the following compounds:

- | | |
|-----------------------------|--|
| (a) Iron(II) nitride | |
| (b) Copper(I) sulfide | |
| (c) Chromium(III) iodide | |
| (d) Palladium(IV) phosphide | |
| (e) Manganese(VI) oxide | |



3.19 Name the following compounds:

- | | |
|-----------------------------|------------------------------|
| (a) Ni_2O_3 | (d) Ni_3P_2 |
| (b) Fe_3N_2 | |
| (c) Cr_2O_3 | (e) Ru_2Se_3 |

3.20 Name the following compounds:

- | | |
|--------------------|---------------------------|
| (a) FeO | (e) MnF_3 |
| (b) CrN | (f) Cu_2C |
| (c) ZnI_2 | |
| (d) CoS | (g) Ag_2O |

3.21 Name or formulate the following ionic (Type II) compounds: (a) Fe_3P_2 (b) Copper(II) iodide (c) Fe_3N_2 (d) Iron(II) sulfide

3.22 Name or formulate the following ionic (Type II) compounds: (a) Fe_2S_3 (b) Gold(III) chloride (c) FeO (d) Vanadium(V) nitride

3.23 Name or formulate the following ionic (Type II) compounds: (a) FeI_2 (b) Lead(IV) sulfide (c) FeBr_2

3.24 Name or formulate the following ionic (Type II) compounds: (a) Manganese(IV) oxide (b) FeCl_2 (c) Copper(I) oxide

ACIDS AND HYDROXIDES

3.25 Name or formulate the following acids or bases: (a) HCl (b) Hydrofluoric Acid (c) $\text{Mg}(\text{OH})_2$

3.26 Name or formulate the following acids or bases: (a) Sulfuric Acid (b) H_2CO_3 (c) Lithium hydroxide

3.27 From the following chemicals identify acids and bases: (a) KOH (b) LiOH (c) CH_3OH

3.28 From the following chemicals identify acids and bases: (a) H_2SO_3 (b) NH_3 (c) $\text{Ca}(\text{OH})_2$

3.29 From the following chemicals identify hydrcids and oxoacids: (a) HF (b) H_2SO_3 (c) H_2S

3.30 From the following chemicals identify hydrcids and oxoacids: (a) H_3BO_3 (b) HCl (c) HI

3.31 Identify the redox number of the central atom of the following oxoacids: (a) H_2CrO_4 (b) $\text{H}_2\text{Cr}_2\text{O}_7$ (c) HMnO_4

3.32 Identify the redox number of the central atom of the following oxoacids: (a) H_2MnO_4 (b) HReO_3 (c) H_2SiO_3

3.33 Identify the most oxidized acid:

- (a) H_3AsO_4 or H_3AsO_3 (b) H_2XeO_4 or H_4XeO_6

3.34 Identify the most reduced acid:

- (a) H_2RuO_4 or HRuO_4 (b) HTcO_4 or H_2TcO_4

3.35 Identify the most oxidant acid:

- (a) H_2CrO_4 or $\text{H}_2\text{Cr}_2\text{O}_7$ (b) HNO_3 or HNO_4

3.36 Identify the most oxidant acid:

- (a) $\text{H}_2\text{S}_2\text{O}_6$ or H_2SO_4 (b) H_2SeO_4 or H_2SeO_3

NAMING OF COMPLEX SALTS AND COMMON CHEMICALS

3.37 Name or formulate the following oxoanions:

- (a) ClO_4^- (b) PO_4^{3-} (c) SO_4^{2-} (d) CO_3^{2-} (e) NO_3^- (f) CrO_4^{2-} (g) BO_3^{3-}

3.38 Name or formulate the following (Type I) oxosalts: (a) $\text{Mg}(\text{NO}_3)_2$ (b) Sodium permanganate (c) KMnO_4 (d) Calcium carbonate (e) Li_3PO_4

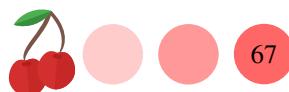
3.39 Name or formulate the following (Type I) oxosalts: (a) Lithium sulfate (b) Na_2CrO_4 (c) Lithium sulfite (d) $\text{Cs}_2\text{Cr}_2\text{O}_7$ (e) Calcium sulfate

3.40 Name or formulate the following compounds:

- (a) Na_2SO_4 (b) KNO_3 (c) CaCO_3 (d) $\text{Ca}(\text{NO}_2)_2$ (e) SrSO_3

3.41 Combine the following ions:

- | | |
|--|--|
| (a) Na^+ + PO_4^{3-} | (d) Ca^{2+} + CO_3^{2-} |
| (b) Li^+ + MnO_4^- | (e) Cs^+ + $\text{Cr}_2\text{O}_7^{2-}$ |
| (c) Mg^{2+} + NO_3^- | (f) K^+ + BO_3^{3-} |



3.42 Combine the following polyatomic ions:

- (a) $\text{Na}^+ + \text{NO}_3^-$ (d) $\text{Ca}^{2+} + \text{CO}_3^{2-}$
(b) $\text{Na}^+ + \text{CO}_3^{2-}$ (e) $\text{Ca}^{2+} + \text{PO}_4^{3-}$
(c) $\text{Na}^+ + \text{PO}_4^{3-}$

3.43 Name or formulate the following (Type II) oxosalts: (a) $\text{Cr}_2(\text{SO}_4)_3$ (b) zinc(II) carbonate (c) $\text{Fe}(\text{MnO}_4)_3$

3.44 Name or formulate the following (Type II) oxosalts: (a) cobalt(III) carbonate (b) $\text{Fe}(\text{ClO}_4)_3$ (c) zinc(II) carbonate

3.45 Name or formulate the following hydrosalts: (a) NaHCO_3 (b) Calcium Hydrogencarbonate
(c) $\text{Al}(\text{HSO}_4)_3$

3.46 Name or formulate the following hydrosalts:
(a) Sodium dihydrogenphosphate (b) LiH_2PO_4 (c) Silver monohydrogenphosphate

3.47 Name or formulate the following hydrates:
(a) $\text{Al}_2(\text{SO}_4)_3 \cdot 3 \text{H}_2\text{O}$ (b) Silver phosphate dihydrate

3.48 Name or formulate the following hydrates:
(a) $\text{KMnO}_4 \cdot 4 \text{H}_2\text{O}$ (b) Lithium sulfate tetrahydrate

3.49 Name or formulate the following compounds:
(a) MgSO_4 (b) $\text{Ni}(\text{SO}_4)_3$ (c) Cobalt(II) nitrate
(d) Cobalt(II) sulfate dihydrate (e) KHCO_3

3.50 Name or formulate the following compounds:
(a) $\text{Ca}(\text{NO}_3)_2$ (b) $\text{Ca}(\text{HCO}_3)_2$ (c) Nickel(II) sulfate
(d) Nickel(II) sulfate tetrahydrate (e) NaH_2PO_4

3.51 Name or formulate the following compounds:
(a) MnSO_4 (b) CuNO_3 (c) $\text{Cr}_2(\text{CO}_3)_3$ (d) $\text{V}(\text{NO}_2)_2$
(e) FeSO_3

3.52 Name or formulate the following pairs or ions:
(a) carbonate and monohydrogencarbonate (b) sulfate and monohydrogensulfate (c) cromate and monohydrogenchromate (d) phosphate and dihydrogenphosphate
(e) phosphate and monohydrogenphosphate (f) borate and dihydrogenborate



Ch. 4. The Mole and Chemical Reactions

WHEN we buy eggs in the store, we buy them by the dozen, and the word dozen actually refers to the number twelve. Similarly, when we measure substances in a chemistry lab we measure them by the mole. This chapter will introduce the idea of mole and you will learn how to relate moles of a chemical to mass using a property called the molecular mass. This chapter also introduces chemical reactions. Chemicals react with each others and a chemical reaction is written in the form an equations. In this chapter you will learn how to balance those equations in order to predict the amount of chemicals produced.

4.1 The mole

Some of the terms you use in your everyday life refer to a number as shown in Figure 4.1. For example, you buy a pair of socks—two socks—or you buy a dozen of eggs from the grocery store—twelve eggs—and sometimes you buy a case of beer—24 cans. In a chemistry laboratory, we normally do not weigh small numbers of molecules of a chemical. In chemistry, molecules are counted by the mole, and the term mole—abbreviated as mol—refers to the 6.022×10^{23} number. For example, a mol of CO molecules contains 6.022×10^{23} molecules of CO, and a mol of water molecules contains 6.022×10^{23} molecules of water. This is because the word mole means the number 6.022×10^{23} , similarly as the word pair means the number two. The number 6.022×10^{23} is called Avogadro's number, about Amedeo Avogadro, the Italian physicist who coined the term. In chemistry labs, chemicals are often measured by weight. In this section, we will show how to convert moles into weight—into grams—by using a property called molecular weight. Finally, mind that the term mol and molecule even if they look similar they are not. Molecule refers to a combination of atoms and mole refers to a large number of molecules. As a note, the abbreviation of the mole is mol, and for example, we will say seven mol of H₂O.

From moles to molecules One mole of molecules contains 6.022×10^{23} molecules. This is because the term mole refers to Avogadro's number. Hence we can use the following unit equivalency:

$$1\text{mol of H}_2\text{O} = 6.02 \times 10^{23} \text{molecules of H}_2\text{O}$$

or a conversion factor to transform moles into molecules or molecules into moles as well:

$$\frac{1\text{mol of H}_2\text{O}}{6.02 \times 10^{23}\text{molecules of H}_2\text{O}} \text{ or } \frac{6.02 \times 10^{23}\text{molecules of H}_2\text{O}}{1\text{mol of H}_2\text{O}}$$



For example: how many molecules are there in 3 mol of H₂O? To calculate the number of molecules of H₂O in 3 moles of H₂O, (moles → molecules) you need to set up a conversion factor, starting with the given information (3 moles) and using the mol-to-molecule conversion factor with mol on the bottom:

$$3 \text{ moles of H}_2\text{O} \times \frac{6.02 \times 10^{23} \text{ molecules of H}_2\text{O}}{1 \text{ mol of H}_2\text{O}} = 1.80 \times 10^{24} \text{ molecules of H}_2\text{O}$$

If you need to convert molecules to moles (molecules → moles), you just need to follow the same procedure, using the conversion factor between mol-to-molecule with molecules in the bottom. For example 3×10^{20} H₂O molecules equals to 4.98×10^{-4} moles of H₂O as

$$3 \times 10^{20} \text{ molecules of H}_2\text{O} \times \frac{1 \text{ mole of H}_2\text{O}}{6.02 \times 10^{23} \text{ molecules of H}_2\text{O}} = 4.98 \times 10^{-4} \text{ moles of H}_2\text{O}$$

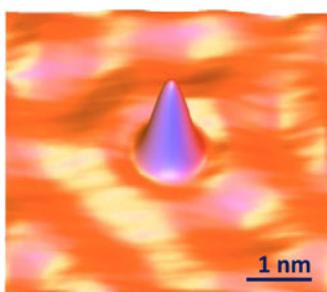
From moles to atoms Molecules are made of atoms, and for example, the CO₂ molecule contains an atom of C and two atoms of O. To convert from molecules to atoms (molecules → atoms) you need to use the coefficients in the molecular formula. For example, a H₂O molecule contains an atom of O and two atoms of H, and hence the relation between water molecules and H and O atoms is:

$$\frac{1 \text{ molecule of H}_2\text{O}}{1 \text{ atom of O}} \text{ and } \frac{1 \text{ molecule of H}_2\text{O}}{2 \text{ atoms of H}}$$

To convert from moles into atoms (moles → atoms) you need to use a two-step process in a single line. First, you convert from moles into molecules, to then convert molecules into atoms. For example, 3 moles of H₂O contains 1.6×10^{24} H atoms, as:

$$3 \text{ moles of H}_2\text{O} \times \frac{6.02 \times 10^{23} \text{ molecules of H}_2\text{O}}{1 \text{ mole of H}_2\text{O}} \times \frac{2 \text{ H atoms}}{1 \text{ molecule of H}_2\text{O}} = 1.6 \times 10^{24} \text{ atoms of H}$$

▼Molecules are counted by the mole



▼Eggs are bought by the dozen



▼Socks are bought as pairs



▼A ream of paper contains 500 sheets



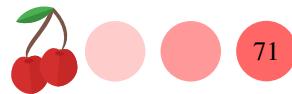
▼A six-pack contains 6 beers



▼A gross is a dozen of dozens



Figure 4.1 Collections of items and their name

**Sample Problem 35**

Calculate: (a) the number of CuO molecules in 3.4 moles of CuO; (b) the number of moles of CO in 5×10^{20} CO molecules

SOLUTION

(a) 3.4 moles of CuO equals to 2.05×10^{22} molecules of CuO as:

$$3.4 \text{ moles of CuO} \times \frac{6.022 \times 10^{23} \text{ molecules of CuO}}{1 \text{ mole of CuO}} = 2.05 \times 10^{24} \text{ molecules of CuO}$$

(b) 5×10^{20} CO molecules equals to 8.3×10^{-4} moles of CO, as

$$5 \times 10^{20} \text{ CO molecules} \times \frac{1 \text{ mole of CO}}{6.022 \times 10^{23} \text{ CO molecules}} = 8.3 \times 10^{-4} \text{ moles of CO}$$

◆ STUDY CHECK

Calculate the number of C, H, N and O atoms in 3.5 moles of caffeine ($C_8H_{10}N_4O_2$).

The following example shows how to relate atoms and moles.

Sample Problem 36

Calculate the number of O atoms in 4.5 moles of NO_2 .

SOLUTION

(c) 4.5 moles of NO_2 contains 5.4×10^{24} O atoms, as

$$4.5 \text{ moles of } NO_2 \times \frac{6.022 \times 10^{23} NO_2 \text{ molecules}}{1 \text{ mole of } NO_2} \times \frac{2 \text{ O atoms}}{1 NO_2 \text{ molecule}} = 5.4 \times 10^{24} \text{ O atoms}$$

▼The molecular mass of cinnamic acid ($C_9H_8O_2$), used in the manufacture of flavors, is $148.16 \frac{g}{mol}$



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▼Car batteries contain sulfuric acid (H_2SO_4), a corrosive chemical with a molar mass of $96.07 \frac{g}{mol}$



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▼Ammonia smelling salts ($(NH_4)_2CO_3$, MW=96g/mol) were historically employed to wake up injured athlete during a sport game.



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▼Acetic acid is an organic acid with molar mass $60g/mol$



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4.2 Converting moles into grams and into atoms

A standard way to measure chemicals in the lab is by weight. We can weigh different quantities and the larger the quantity the larger the weight. For a chemical, the weight of a mole is called the molar (or molecular) weight. For example, if we weigh a mole of water (H_2O) we will be weighing 18 grams of water, or if you weigh a mole of table salt ($NaCl$) the scale will show 58 grams. In this section, you will learn how to calculate the molar mass of a chemical and how to use this property to convert from weight to moles (and moles to weight).

Molar mass of a chemical Chemicals are made of atoms, and each atom has a specific atomic weight (AW) listed in the periodic table. For example, the atomic weight of Na is 23 grams whereas the atomic weight of Cl is 35 g. The weight of all the atoms of a molecule is called the molecular weight (we call this also molar weight or MW). For example, the molecular weight of $NaCl$ is 58 g, as the weight of Na and Cl is 23 and 35g. Another example would be water, H_2O with a molecular weight of 18g—as the atomic weight of H and O is 1 and 16 g, respectively, and the molecule has two



H atoms. The units for molecular weight is $\frac{g}{mol}$, also written as g/mol . To compute the molar mass of a molecule you need to break down the molecule into atoms using the coefficients in the formula. For example, the formula for vinegar is $C_2H_4O_2$ which means a vinegar molecule contains 2C, 4H and 2O atoms. If you add the atomic masses of 2C, 4H, and 2O you will get $60g/mol$. If the chemical formula has a parenthesis, you need to open up the parenthesis to calculate the total number of atoms. As an example, $Ca(NO_3)_2$ contains 1Ca, 2N, and 6O, and its molar mass is $164.09g/mol$.

Sample Problem 37

Calculate: (a) The atomic weight of Mg; (b) the molecular mass of sulfuric acid, H_2SO_4

SOLUTION

(a) According to the periodic table the atomic weight (AW) of Mg is $24.31g/mol$. (b) The molar mass of H_2SO_4 is the result of adding the atomic masses of 2H ($AW=1g/mol$) atoms, 1 S ($AW=32g/mol$) and 4O ($AW=16g/mol$) atoms, that gives $98.08g/mol$.

◆ STUDY CHECK

Calculate the molar mass of glucose $C_6H_{12}O_6$

From moles to grams The molar mass is used to convert moles to grams or grams to mol. For example, the molar mass of water is $18g/mol$. This means:

$$1 \text{ mole of H}_2\text{O} = 18 \text{ g of H}_2\text{O}$$

that is the same as

$$\frac{1 \text{ mole of H}_2\text{O}}{18 \text{ grams of H}_2\text{O}} \text{ or } \frac{18 \text{ grams of H}_2\text{O}}{1 \text{ mole of H}_2\text{O}}$$

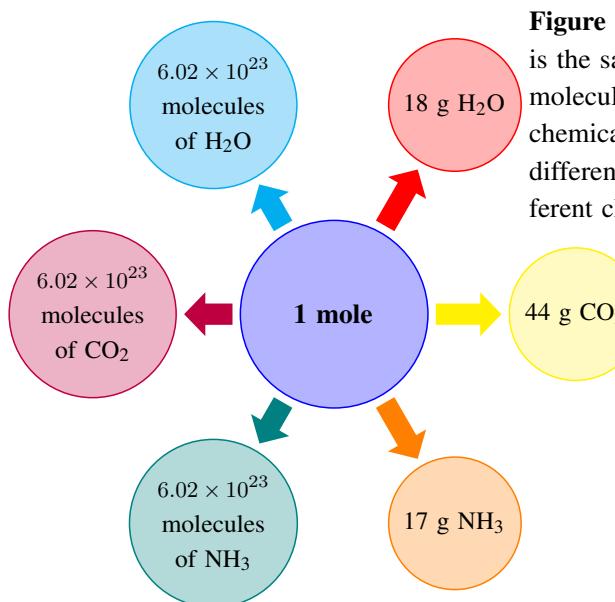
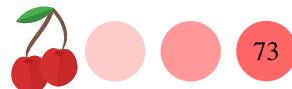


Figure 4.2 A mole is the same number of molecules for different chemicals, while being different weights for different chemicals.

**Sample Problem 38**

Smelling salts ($(\text{NH}_4)_2\text{CO}_3$) are chemicals used to arouse consciousness. These are used by pro athletes to get into the zone before a game. How many moles of salt do you have in 100 grams of these salts?

SOLUTION

We first need to calculate the molar mass of $(\text{NH}_4)_2\text{CO}_3$, a chemical with 2N, 8H, 1C and 3O atoms. The molar mass hence would be: $2 \times 14 + 8 \times 1 + 1 \times 12 + 3 \times 16 = 96 \text{ g/mol}$. In order to calculate the moles given the gram, you need to use the molar mass as a conversion factor:

$$\frac{100 \text{ g of } (\text{NH}_4)_2\text{CO}_3}{96 \text{ g of } (\text{NH}_4)_2\text{CO}_3} \times \frac{\text{moles of } (\text{NH}_4)_2\text{CO}_3}{\text{g of } (\text{NH}_4)_2\text{CO}_3} = 1.04 \text{ moles of } (\text{NH}_4)_2\text{CO}_3$$

◆ STUDY CHECK

Calculate the MW of table salt (NaCl) and the grams in 20 moles of this salt.

From grams to atoms In the previous sections, we covered how to convert grams to moles, moles to molecules, or molecules to atoms. You can follow the diagram below to switch from one of these properties (atoms, molecules, moles, grams) to another. For example, if you want to convert grams into moles, you will only need one step and you will only have to use a single property: the molar mass. Differently, if you need to convert grams into molecules you will have to use two different steps and use two different properties: the molar mass and Avogadro's number.

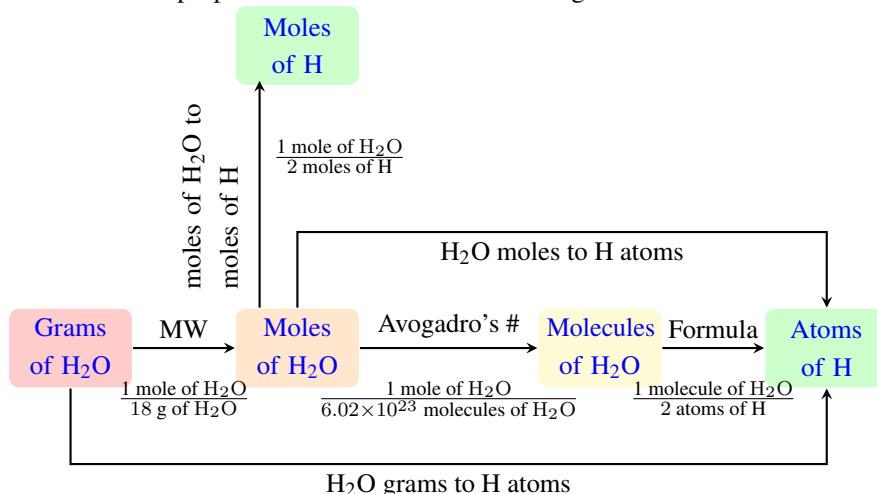


Figure 4.3 Diagrams relating grams, moles of molecules, moles of atoms, atoms and molecules.

Sample Problem 39

Convert 10 grams of ammonia (NH_3 , MW=17 g/mol) into H atoms.

SOLUTION

We will have to do this conversion in three different steps. First we will go from grams to moles, then from moles to molecules to finally transform molecules



▼ A termite reaction between iron(III) oxide and Al: $\text{Fe}_2\text{O}_3 + 2\text{Al} \longrightarrow 2\text{Fe} + \text{Al}_2\text{O}_3$



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▼ An image of the combustion of Mg: $2\text{Mg(s)} + \text{O}_2\text{(g)} \longrightarrow 2\text{MgO(s)}$



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▼ Iron rust is the result of a combination reaction: $4\text{Fe} + 2\text{O}_2 \longrightarrow 2\text{Fe}_2\text{O}_3$



© wikipedia

▼ Wood burning is a combustion reaction



© Pngimg

into atoms:

$$10\text{ g of NH}_3 \times \frac{1 \text{ mole of NH}_3}{17 \text{ g of NH}_3} \times \frac{6.022 \times 10^{23} \text{ NH}_3 \text{ molecules}}{1 \text{ mole of NH}_3} \times \frac{3 \text{ H atoms}}{1 \text{ NH}_3 \text{ molecule}} = 1.8 \times 10^{24} \text{ H atoms}$$

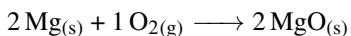
◆ STUDY CHECK

Methane is a chemical used as a fuel. Calculate how many grams of methane CH_4 contains 5×10^{25} H atoms.

4.3 Chemical reactions

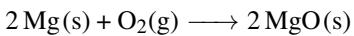
When we eat we burn food with molecular oxygen (O_2) to produce carbon dioxide and water. Similarly, when we start the engine of the car to go to work, gasoline burns to produce the same chemicals: CO_2 and H_2O . These are two examples of chemical reactions, but there are many other examples. Nitrogen from the air reacts with hydrogen to produce ammonia, a common chemical used in the production of fertilizers. This section covers the basics of chemical reactions. You will learn how to balance reactions and how to classify reactions.

Simple chemical reactions Magnesium is a metal that reacts with oxygen to produce magnesium oxide. Magnesium is solid Mg(s) whereas oxygen is gas and contains two oxygen atoms per molecule $\text{O}_2\text{(g)}$. Magnesium oxide, the result of the reaction, is solid MgO(s) . The reaction between magnesium and oxygen to produce magnesium oxide



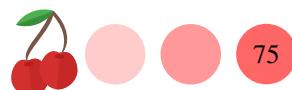
Mg and O_2 combine—that is why we use a plus sign—to produce MgO —we use an arrow to indicate that a chemical is being produced. Also, the symbols (s) or (g) indicates solid or gas state. The reactants are located before the arrow and the products are after the arrow. The numbers in front of the reactants and products (2, 1 and 2) are called stoichiometric coefficients, and we will talk more about them in the following sections.

Reading a chemical reaction Chemical reactions can be read in words. To read a chemical reaction you need to connect the reactants with the word “react” and then use the words “to produce” and after that, you need to read the products. The numbers in front of the reactants and products represent the number of moles, and you need to include those numbers in the reading. For example, the following reaction

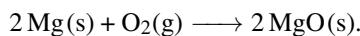


should be read as: “two moles of Mg react with one mole of O_2 to produce two moles of MgO ”.

Balanced chemical reactions Chemical reactions contain molecules, which are made of atoms. Some chemical reactions are balanced, and others need to be balanced. To identify a balanced reaction, you should use the stoichiometric coefficients and the indexes in the molecular formulas to break down the reactants and products



into atoms. In a balanced chemical reaction, the atoms of reactants should be the same as the atoms of the products. Consider the following reaction,

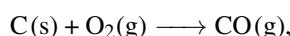


The table below shows all reactants and products in the form of atoms.

$2 \text{Mg(s)} + \text{O}_2\text{(g)} \longrightarrow 2 \text{MgO(s)}$		
Reactants	Products	
2Mg	2Mg	✓
O ₂ =2O	2O	✓

The number of Mg atoms in the reactants and products is the same and equals two. On the other hand, the number of O atoms in the reactants and products is the same, equal to two. For this reason, we say this reaction is *balanced*.

Now consider the following reaction:



The number of C atoms in the reactants and products is the same and equals one. In contrast, the number of O atoms in the reactants and products is not the same, and for this reason, we say this reaction is *not balanced*.

$\text{C(s)} + \text{O}_2\text{(g)} \longrightarrow \text{CO(g)}$		
Reactants	Products	
1C	1C	✓
O ₂ =2O	O	✗

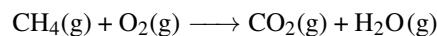
Balancing chemical reactions To balance a reaction, we need to introduce the stoichiometric coefficients that make the number of atoms of reactants and products the same. To balance the number of oxygens, we will multiply CO by two, and that will give us two oxygens and two carbons as well. If we do this, now the carbon atoms of reactants and products will not be the same. We can solve this by multiplying C(s) by two. The following table summarizes the changes we made:

$2 \text{C(s)} + \text{O}_2\text{(g)} \longrightarrow 2 \text{CO(g)}$		
Reactants	Products	
2C	2C	✓
O ₂ =2O	2O	✓

The reaction is now balanced after introducing two stoichiometric coefficients and the number of C and O atoms in the reactant molecules and products is the same.

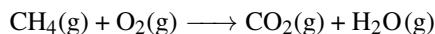
Sample Problem 40

Balance the following reaction:



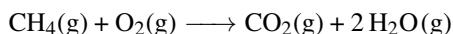
SOLUTION

We will break down each molecule into atoms. In the case of O, both CO₂ and H₂O contain oxygen and hence you will have to combine both oxygen atoms:



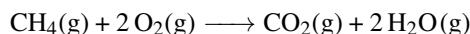
Reactants	Products	
1C	1C	✓
4H	2H	✗
2O	3O	✗

The reaction is not balanced as the number of H and O atoms for the reactants and products is not the same. In order to balance the H, you can multiply by two H_2O , and that will balance H but also affect O.



Reactants	Products	
1C	1C	✓
4H	4H	✓
2O	4O	✗

You can balance O by multiplying O_2 by two. That will give you the final balanced reaction in which all atoms (O, H and C) are the same in the product and reactant molecules.



Reactants	Products	
1C	1C	✓
4H	4H	✓
4O	4O	✓

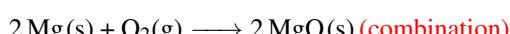
◆ STUDY CHECK

Balance the following reaction: $\text{Fe}_2\text{O}_3(\text{s}) + \text{C}(\text{s}) \longrightarrow \text{Fe}(\text{s}) + \text{CO}(\text{g})$

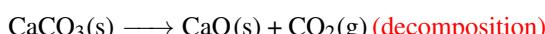
4.4 Five types of reactions

Most chemical reactions can be classified according to five types: combination, decomposition, single replacement, double replacement, and combustion.

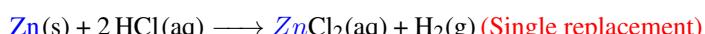
In a *combinations reaction* two reactants combine to generate a product. An example of a combination is the reaction between Mg and oxygen to produce MgO:



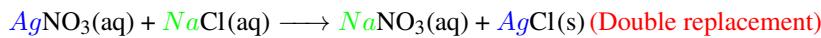
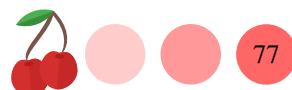
In a *decomposition reaction* a single reactant breaks down into several products. An example of a decomposition reaction is the thermal reaction of CaCO_3 to produce calcium oxide (CaO) and carbon dioxide



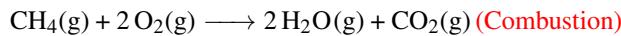
In a single replacement reaction, an element replaces another element in a chemical. An example would be the reaction of Zn with HCl, in which Zn replaces hydrogen:



In a double replacement reaction, the first element in the reacting compounds switches places. An example is the reaction between AgNO_3 and NaCl , in which Ag from AgNO_3 replaces Na in NaCl :

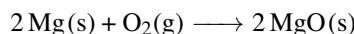


Finally, in a combustion reaction, a carbon-based chemical reacts with oxygen to produce carbon dioxide and water. An example would be the combustion of methane (CH_4):



4.5 Stoichiometry

In the previous section, you learned how to balance a chemical reaction. To do this, you had to find the stoichiometric coefficients that balance the atoms of the reactant and products. In this new section, we will learn how to use those coefficients to predict the amount of product formed. You will also learn how to predict the amount of reactant needed to react with another reactant. We will use the reaction between Mg and oxygen:



in which two moles of Mg and one mole of O_2 produce two moles of MgO. We will refer to this reaction in the following.

Mole-Mole ratio A chemical reaction can be expressed in the form of conversion factors. For example, the mole ratio between Mg (a reactant) and O_2 (another reactant) and between Mg and MgO is:

$$\frac{2 \text{ moles of Mg}}{1 \text{ moles of O}_2} \text{ or } \frac{1 \text{ moles of O}_2}{2 \text{ moles of Mg}} \text{ and } \frac{2 \text{ moles of Mg}}{2 \text{ moles of MgO}} \text{ or } \frac{2 \text{ moles of MgO}}{2 \text{ moles of Mg}}$$

Finally, the mole ratio between O_2 and MgO is:

$$\frac{1 \text{ moles of O}_2}{2 \text{ moles of MgO}} \text{ or } \frac{2 \text{ moles of MgO}}{1 \text{ moles of O}_2}$$

Mole ratios are used, for example, to transform the amount of reactant into the product.

Reactants to products We will calculate how much MgO will be produced from 5 moles of Mg by converting Mg into MgO using the conversion factor between both chemicals. As we want to transform the Mg into MgO we will use the conversion factor with Mg at the bottom of the fraction. This way the units will cancel out to give moles of MgO:

$$5 \cancel{\text{moles of Mg}} \times \frac{2 \text{ moles of MgO}}{2 \cancel{\text{moles of Mg}}} = 5 \text{ moles of MgO.}$$

This result means that 5 moles of Mg will produce 5 moles of MgO.

Reactant to a different reactant Sometimes we will have to calculate how much reactant will be needed to react with another reactant. In those cases, we will use the conversion factor that relates both reactants. If we have 5 moles of Mg and we want to know how much oxygen we need to react with Mg, we will proceed as:

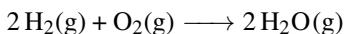
$$5 \cancel{\text{moles of Mg}} \times \frac{1 \text{ mole of O}_2}{2 \cancel{\text{moles of Mg}}} = 2.5 \text{ moles of O}_2.$$

This result means that 2.5 moles of O_2 will react with 5 moles of Mg.



Sample Problem 41

Hydrogen reacts with oxygen to produce water according to the following reaction



Calculate: (a) the number of moles of water produced from 5 moles of H₂; (b) the number of moles of oxygen needed to react with 7 moles of H₂.

SOLUTION

(a) we will first convert 5 moles of H₂ into water:

$$\frac{5 \text{ moles of H}_2}{2 \text{ moles of H}_2} \times \frac{2 \text{ moles of H}_2\text{O}}{2 \text{ moles of H}_2} = 5 \text{ moles of H}_2\text{O},$$

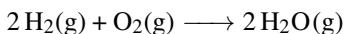
that is: 5 moles of hydrogen produce 5 moles of water. (b) We will now calculate the amount of oxygen needed to react with 7 moles of hydrogen

$$\frac{7 \text{ moles of H}_2}{2 \text{ moles of H}_2} \times \frac{1 \text{ mole of O}_2}{2 \text{ moles of H}_2} = 3.5 \text{ moles of O}_2,$$

that is: 3.5 moles of O₂ will react with 7 moles of H₂.

◆ STUDY CHECK

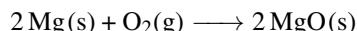
Hydrogen reacts with oxygen to produce water according to the following reaction



Calculate the number of moles of water produced by 4 moles of oxygen.

4.6 Mass calculations

In the previous sections, given the moles of reactants, we learned how to use chemical reactions to predict the amount of product formed. In this section, we will learn how to do the same, but instead of starting with the number of moles, this time, we will work our way starting with a quantity given in grams. We will base the following examples on the reaction of Mg and O₂:

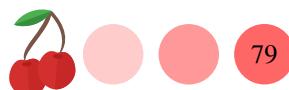


Molar mass review Remember that the molar mass (also known as molecular weight, MW. Atomic weight for the atoms, AW) of a chemical is a property used to convert grams into moles. For example, the molar mass of H₂O is 18 g/mol. If we need to convert 12 grams of water into mols we should do:

$$\frac{12 \text{ g of H}_2\text{O}}{18 \text{ g of H}_2\text{O}} \times \frac{\text{moles of H}_2\text{O}}{1 \text{ mol of H}_2\text{O}} = 0.66 \text{ moles of H}_2\text{O}$$

To use the stoichiometric coefficients from a chemical reaction, the starting quantity must be the moles of a reactant or products. This is because these coefficients are expressed in moles and hence to operate with them you can only use moles.

From grams to moles If we want to calculate the grams of MgO produced from 3 moles of Mg, we will start with the moles of Mg and use a conversion factor that



relates moles of Mg and moles of MgO, locating the moles of Mg on the bottom:

$$3 \cancel{\text{moles of Mg}} \times \frac{2 \text{ moles of MgO}}{2 \cancel{\text{moles of Mg}}} = 3 \text{ moles of MgO.}$$

Now we aim to calculate the number of MgO moles produced from 5 grams of Mg (AW=24g/mol). This time, we will have first to convert the grams of Mg into moles to then use the mole ratio between Mg and MgO:

$$5 \cancel{\text{g of Mg}} \times \frac{1 \cancel{\text{mole of Mg}}}{24 \cancel{\text{g of Mg}}} \times \frac{2 \text{ moles of MgO}}{2 \cancel{\text{moles of Mg}}} = 0.21 \text{ moles of MgO.}$$

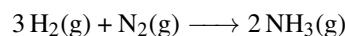
From grams to grams We want to answer the following question: we have 6 moles of Mg (AW=24g/mol) and we want to calculate the mass of MgO(MW=40g/mol) produced. The importance of this type of calculation is based on the fact that in a chemistry laboratory chemicals are normally weighted in grams. To answer this example, we will start with the grams of Mg and convert this quantity to moles of Mg using the atomic mass. After that, we will use the mole ratio between Mg and MgO to calculate the moles of MgO. At this point, we will finish the calculation by converting the moles of MgO into grams using its molecular weight:

$$5 \cancel{\text{grams of Mg}} \times \frac{1 \cancel{\text{mole of Mg}}}{24 \cancel{\text{grams of Mg}}} \times \frac{2 \cancel{\text{moles of MgO}}}{2 \cancel{\text{moles of Mg}}} \times \frac{40 \text{ grams of MgO}}{1 \cancel{\text{mole of MgO}}} \\ = 10 \text{ grams of MgO.}$$

Overall, we have that 5 grams of Mg will produce 10 grams of MgO.

Sample Problem 42

For the reaction of hydrogen and nitrogen to produce ammonia (NH₃):



Calculate: (a) the number of moles of NH₃ produced from 10 grams of hydrogen (MW=2g/mol); (b) Calculate the number of grams of NH₃ (MW=17g/mol) produced from 10 grams of nitrogen (MW=28g/mol)

SOLUTION

(a) You will solve this problem in a single line by using two steps: first convert the grams of hydrogen to moles, to then convert the moles of hydrogen into ammonia:

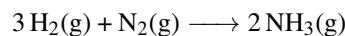
$$10 \cancel{\text{grams of H}_2} \times \frac{1 \cancel{\text{mole of H}_2}}{2 \cancel{\text{grams of H}_2}} \times \frac{2 \text{ moles of NH}_3}{3 \cancel{\text{moles of H}_2}} = 3.33 \text{ moles of NH}_3.$$

In other words, 10 grams of hydrogen produce 3.33 moles of ammonia. (b) To solve this question, we will use one additional step in order to convert the moles of ammonia into grams:

$$10 \cancel{\text{grams of N}_2} \times \frac{1 \cancel{\text{mole of N}_2}}{28 \cancel{\text{grams of N}_2}} \times \frac{2 \cancel{\text{moles of NH}_3}}{1 \cancel{\text{mole of N}_2}} \times \frac{17 \text{ grams of NH}_3}{1 \cancel{\text{mole of NH}_3}} \\ = 12.14 \text{ grams of NH}_3.$$

◆ STUDY CHECK

For the reaction of hydrogen and nitrogen to produce ammonia (NH₃):



Calculate the number of grams of nitrogen needed to react with 3 grams of hydrogen to produce ammonia.



4.7 Percent yield

Often, reactions do not fully proceed to completion. Fewer amounts of products are obtained when a specific quantity of a chemical is expected from a reaction. The percent yield tells how much of the final chemical is produced. The larger the yield the larger the amount of products generated and therefore, less waste is generated. At the same time, when mixing two reactants sometimes leftovers remain. In other words, sometimes there is a reagent that limits the reaction and an excess reagent. This section will cover the very important ideas of percent yield and limiting (or excess) reagents.

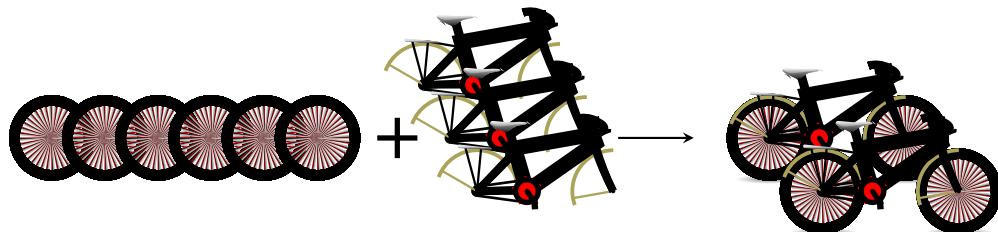
Percent yield Chemical reactions are less than perfect as the starting material does not fully convert into products. Furthermore, side reactions often occur in competition with the main reaction generating byproducts. The theoretical yield is the number of products one will expect in a hypothetically perfect chemical reaction, while the actual yield is the amount of product that is produced. Therefore, the percent yield is just the fraction between the actual yield and the theoretical yield in percent form:

$$\% \text{ Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

To compute the percent yield, we need the theoretical yield, which is the amount of product that will be produced following the rules of stoichiometry, and the actual yield, normally known in an experiment from lab measurements. Look at the scenario below: we need two wheels and a body to ensemble a bike. We can think about the bike production yield based on the starting materials we have.

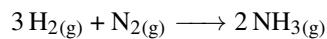


If we have three pairs of wheels and three bodies and we only produce two bikes, the yield will be 67%.



Sample Problem 43

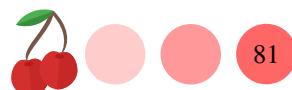
Ammonia is produced by reacting molecular nitrogen and molecular hydrogen following the reaction:



What is the percent yield of ammonia if 4 moles of hydrogen gives 2 moles of ammonia.

SOLUTION

We will first compute the theoretical yield, that is the moles of ammonia pro-



duced from 4 moles of hydrogen:

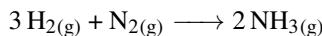
$$4 \text{ moles of H}_2 \times \frac{2 \text{ moles of NH}_3}{3 \text{ moles of H}_2} = 2.66 \text{ moles of NH}_3.$$

Hence the theoretical yield is 2.66 moles of NH₃, and the actual yield given in the problem is 2 moles of NH₃. The actual yield is smaller than the theoretical yield. That is reasonable as the moles of ammonia produced in the real experiment should always be smaller than the amount of ammonia produced in theory. To calculate the percent yield we use the formula:

$$\text{Percent Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100 = \frac{2}{2.66} \times 100 = 75.18\%$$

STUDY CHECK

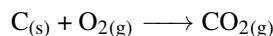
Ammonia is produced by reacting molecular nitrogen and molecular hydrogen following the reaction:



Calculate the percent yield of ammonia if 1 moles of nitrogen gives 1.5 moles of ammonia

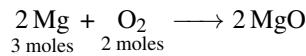
4.8 Limiting reagent

Let us consider the reaction between solid carbon and molecular oxygen to produce CO₂:



This reaction should be read as “one mole of carbon reacts with one mole of molecular oxygen to produce one mole of carbon dioxide”. Mind that to produce one mole of CO₂ you need one mole of C and one mole of molecular oxygen. Now, what would happen if you mix one mole of carbon with 0.5 moles of oxygen? In this scenario, when the 0.5 moles of oxygen are consumed the reaction will stop; half a mole of carbon dioxide will be formed and half a mole of C will remain. Differently, no oxygen will remain and the whole 0.5 moles will consume. We say that C is the excess reactant and oxygen is the limiting reactant. Often a reaction will be accompanied by the reagent quantities and you will have to identify the limiting reagent. This reagent will limit the amount of product formed, and hence, any stoichiometric calculation aimed to predict the amount of product formed should be based on the limiting reagent and never on the excess reagent. Next, we will explain how to systematically identify the limiting reagent.

Identify the limiting reagent Consider the following reaction, in which 3 moles of Mg react with 2 moles of oxygen to produce magnesium oxide:



To identify the limiting reagent, we will choose one of the given reagent quantities and calculate the moles of the other reagent needed (we will call this n_{needed}). For example, if we choose to start with 3 moles of Mg, the amount of oxygen needed to react with



this quantity will be:

$$n_{\text{needed}}^{\text{O}_2} = 3 \frac{\text{moles of Mg}}{\text{2 moles of Mg}} \times \frac{1 \text{ moles of O}_2}{\text{2 moles of Mg}} = 1.5 \text{ moles of O}_2.$$

This means that to react with 3 moles of Mg you need $n_{\text{needed}}^{\text{O}_2} = 1.5$ moles of oxygen. On the other hand, you have two moles of oxygen ($n_{\text{given}}^{\text{O}_2} = 2$), and that is more than what you need to react with the 3 moles of Mg. Hence,

$$n_{\text{needed}}^{\text{O}_2} < n_{\text{given}}^{\text{O}_2}$$

oxygen is the excess reagent and Mg is the limiting reagent. The leftovers will be:

$$n_{\text{left}}^{\text{O}_2} = |n_{\text{needed}}^{\text{O}_2} - n_{\text{given}}^{\text{O}_2}| = 0.5 \text{ moles of O}_2$$

Let us reinforce the idea of limiting reagents with the scenario below. If we have three wheels and two bodies, the number of wheels limits bike production.

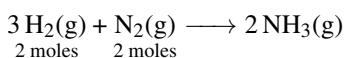


Differently, if we have three wheels and one body, then the body of the bikes limit production.



Sample Problem 44

In the synthesis of ammonia (NH_3):



you mix 2 moles of hydrogen with 2 moles of nitrogen. Identify the limiting and excess reagents and indicate the moles of leftover remaining.

SOLUTION

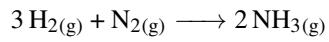
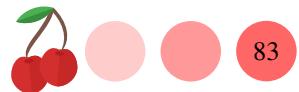
We will choose one of the reagents, for example the two moles of hydrogen, and calculate the amount of nitrogen needed to react with this amount of oxygen:

$$2 \frac{\text{moles of H}_2}{\text{3 moles of H}_2} \times \frac{1 \text{ moles of N}_2}{\text{3 moles of H}_2} = 0.66 \text{ moles of N}_2.$$

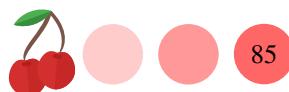
Therefore, to react with 2 moles of hydrogen we need 0.66 moles of nitrogen, and we have 2 moles of nitrogen. This means we have more nitrogen than what we need and hence, nitrogen is the excess reagent and hydrogen the limiting reagent. As we need 0.66 moles of nitrogen and we have 2 moles, 1.33 moles of nitrogen will remain.

❖ STUDY CHECK

In the synthesis of ammonia (NH_3):



you mix 3 moles of hydrogen with 0.5 moles of nitrogen. Identify the limiting and excess reagents and indicate the moles of leftover remaining.



CHAPTER 4

THE MOLE

4.1 Calculate the number of molecules in: (a) 8 moles of CO (b) 10 moles of CO₂

4.2 Calculate the number of molecules in: (a) 4 moles of NH₃ (b) 50 moles of H₂SO₄

4.3 Calculate the number of moles in: (a) 6×10^{23} molecules of NO (b) 5×10^{15} molecules of NaCl (c) 3×10^{27} molecules of MgO

4.4 Calculate the number of moles in: (a) 3.2×10^{21} molecules of H₂O (b) 2×10^{23} molecules of CO₂

4.5 Fill the conversion factor that calculates the final property:

$$10^{24} \text{ molecules of } \cancel{\text{NO}_2} \times \frac{\text{moles of } \text{NO}_2}{\cancel{\text{molecules of } \text{NO}_2}} = \text{moles of } \text{NO}_2.$$

4.6 Fill the conversion factor that calculates the final property:

$$3 \cancel{\text{moles of } \text{NO}} \times \frac{\text{molecules of } \text{NO}}{\cancel{\text{moles of } \text{NO}}} = \text{molecules of } \text{NO}.$$

4.7 Fill the conversion factor that calculates the final property:

$$6 \cancel{\text{moles of } \text{C}_6\text{H}_{12}\text{O}_6} \times \frac{\cancel{}}{\cancel{}} = \text{molecules of } \text{C}_6\text{H}_{12}\text{O}_6.$$

4.8 Fill the conversion factor that calculates the final property:

$$10^{25} \cancel{\text{molecules of } \text{CH}_4\text{N}_2\text{O}} \times \frac{\cancel{}}{\cancel{}} = \text{moles of } \text{CH}_4\text{N}_2\text{O}.$$

ATOMS

4.9 Calculate the molar weight of the following molecules: (a) CO (b) H₂ (c) Fe₂(CO₃)₃

4.10 Calculate the molar weight of the following molecules: (a) NH₃ (b) O₂

4.11 Fill the conversion factor that calculates the final property:

$$4 \cancel{\text{moles of } \text{CO}_2} \times \frac{\text{g of } \text{CO}_2}{\cancel{\text{moles of } \text{CO}_2}} = \text{g of } \text{CO}_2.$$

4.12 Fill the conversion factor that calculates the final property:

$$10 \cancel{\text{g of } \text{NO}} \times \frac{\text{moles of } \text{NO}}{\cancel{\text{g of } \text{NO}}} = \text{moles of } \text{NO}.$$

4.13 Fill the conversion factor that calculates the final property:

$$5 \cancel{\text{moles of } \text{C}_6\text{H}_{12}\text{O}_6} \times \frac{\cancel{}}{\cancel{}} = \text{g of } \text{C}_6\text{H}_{12}\text{O}_6.$$

4.14 Fill the conversion factor that calculates the final property:

$$7 \cancel{\text{g of } \text{CH}_4\text{N}_2\text{O}} \times \frac{\cancel{}}{\cancel{}} = \text{moles of } \text{CH}_4\text{N}_2\text{O}.$$

4.15 Fill the conversion factor that calculates the final property:

$$10^{26} \cancel{\text{molecules of } \text{NO}_2} \times \frac{\text{atoms of } \text{O}}{\cancel{\text{molecules of } \text{NO}_2}} = \text{atoms of } \text{O}.$$



4.16 Fill the conversion factor that calculates the final property:

$$10^{22} \text{ atoms of O} \times \frac{\text{molecules of H}_2\text{O}}{\text{atoms of O}} = \text{molecules of H}_2\text{O}$$

4.17 Fill the conversion factor that calculates the final property:

$$6 \text{ molecules of C}_6\text{H}_{12}\text{O}_6 \times \frac{\text{atoms of C}}{\text{molecules of C}_6\text{H}_{12}\text{O}_6} = \text{atoms of C.}$$

4.18 Fill the conversion factor that calculates the final property:

$$10^{21} \text{ atoms of N} \times \frac{\text{molecules of CH}_4\text{N}_2\text{O}}{\text{atoms of N}} = \text{molecules of CH}_4\text{N}_2\text{O.}$$

4.19 Answer the following questions: (a) Calculate the number of C atoms in 3 moles of C₁₀H₁₄N₂? (b) Calculate the number of H atoms in 3 moles of C₁₀H₁₄N₂? (c) Calculate the number of N atoms in 3 moles of C₁₀H₁₄N₂

4.20 Answer the following questions: (a) How many grams are there in 4 moles of C₆H₁₂O₆? (b) How many C atoms are there in 3 moles of C₆H₁₂O₆? (c) How many O atoms are there in 3 moles of C₆H₁₂O₆?

4.21 Calculate the molar weight of the following molecules: (a) benzene, C₆H₆ (b) Carbon disulfide, CS₂ (c) Nitrogen tetroxide, N₂O₄

4.22 Calculate the molar weight of the following molecules: (a) Sulfur dioxide, SO₂ (b) Unsymmetrical dimethyl hydrazine, (CH₃)₂NNH₂ (c) Dimethyl sulfide, (CH₃)₂S

4.23 Fill the conversion factor that calculates the final property, given that the molar mass of C₂H₆ is 30g/mol:

$$7 \times 10^{21} \text{ atoms of C} \times \frac{\text{molecules of C}_2\text{H}_6}{\text{atoms of C}} = \text{molecules of C}_2\text{H}_6$$

4.24 Fill the conversion factor that calculates the final property, given that the molar mass of C₂H₆ is 30g/mol:

$$5 \times 10^{25} \text{ atoms of H} \times \frac{\text{molecules of C}_2\text{H}_6}{\text{atoms of H}} \times \frac{\text{g of C}_2\text{H}_6}{\text{molecules of C}_2\text{H}_6} = \text{g of C}_2\text{H}_6$$

CHEMICAL REACTIONS

4.25 Balance the following reactions: (a) P₄(s) + O₂(g) → P₄O₁₀(s) (b) Al(s) + O₂(g) → Al₂O₃(s)

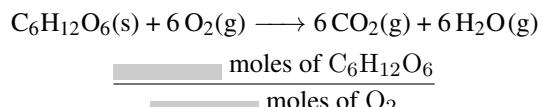
4.26 Balance the following reactions: (a) FeS(s) + O₂(g) → Fe₂O₃(s) + SO₂(g) (b) NH₃(g) + O₂(g) → NO(g) + H₂O(g)

4.27 Classify next reaction as combination, decomposition, single replacement, double replacement, or combustion: (a) Pb_(s) + FeSO_{4(s)} → PbSO_{4(s)} + Fe_(s) (b) C₆H_{12(g)} + 9 O_{2(g)} → 6 CO_{2(g)} + 6 H₂O_(g) (c) 2 RbNO_{3(aq)} + BeF_{2(aq)} → Be(NO₃)_{2(aq)} + 2 RbF_(aq)

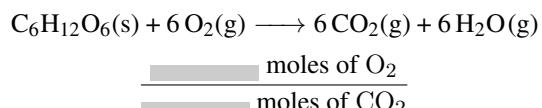
4.28 Balance the following reactions: (a) H_{2(g)} + Br_{2(g)} → HBr_(g) (b) C_(g) + O_{2(g)} → CO_(g) (c) O_{3(g)} → O_{2(g)} (d) NH₄NO_{2(aq)} → N_{2(g)} + H₂O_(l) (e) Na₃PO_{4(aq)} + MgCl_{2(aq)} → Mg₃(PO₄)_{2(aq)} + NaCl_(aq)

STOICHIOMETRY AND MASS CALCULATIONS

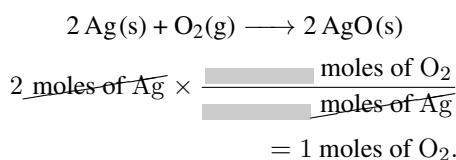
4.29 Fill the mole ratio for the following reaction:

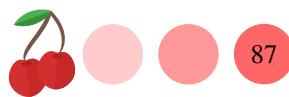


4.30 Fill the mole ratio for the following reaction:

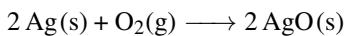


4.31 Fill the conversion factor that calculates the moles of oxygen needed to react with 2 moles of Silver producing AgO:



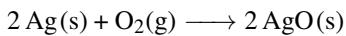


4.32 Fill the conversion factor that calculates the moles of AgO produced from 2 moles of Silver:



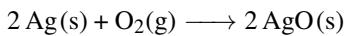
$$\frac{2 \text{ moles of Ag}}{\text{moles of Ag}} \times \frac{\text{moles of AgO}}{\text{moles of Ag}} = 2 \text{ moles of AgO.}$$

4.33 Fill the conversion factor that calculates the moles of AgO produced from 10 moles of oxygen:



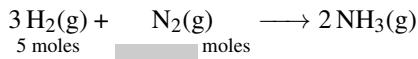
$$\frac{10 \text{ moles of O}_2}{\text{moles of O}_2} \times \frac{\text{moles of AgO}}{\text{moles of O}_2} = 20 \text{ moles of AgO.}$$

4.34 Fill the conversion factor that calculates the moles of AgO produced from 5 moles of oxygen:

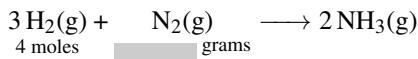


$$\frac{5 \text{ moles of O}_2}{\text{moles of O}_2} \times \frac{\text{moles of AgO}}{\text{moles of O}_2} = 10 \text{ moles of AgO.}$$

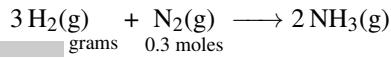
4.35 Calculate how many moles of nitrogen are needed to react with 5 moles of hydrogen, to produce ammonia:



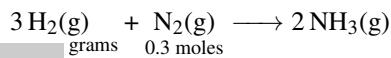
4.36 Calculate the number of grams of nitrogen needed to react with 4 moles of hydrogen, to produce ammonia:



4.37 Calculate the number of grams of hydrogen needed to react with 0.3 moles of nitrogen, to produce ammonia:

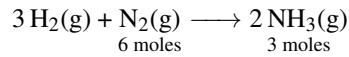


4.38 Calculate the number of grams of hydrogen needed to react with 5 moles of nitrogen, to produce ammonia:

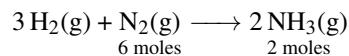


PERCENT YIELD AND LIMITING REAGENT

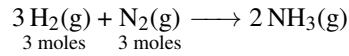
4.39 Six moles of nitrogen gas react to produce three moles of ammonia according to the following reaction:



4.40 Six moles of nitrogen gas react to produce two moles of ammonia according to the following reaction:

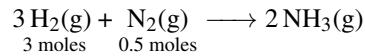


4.41 We mix three moles of hydrogen gas with three moles of nitrogen gas.



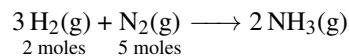
Calculate the limiting reagent.

4.42 We mix three moles of hydrogen gas with half a mole of nitrogen gas.



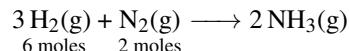
Calculate the limiting reagent.

4.43 We mix two moles of hydrogen gas with five moles of nitrogen gas.



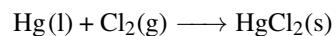
Calculate the limiting reagent.

4.44 We mix six moles of hydrogen gas with two moles of nitrogen gas.



Calculate the limiting reagent.

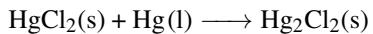
4.45 Liquid mercury reacts with gas chlorine to produce mercury(II) choride, a white solid:



In an experiment, 5-mL of mercury (AW=200.59g/mol) with density 5g/mL, reactants with 4-g of chlorine to produce 6g of HgCl₂. What is the percent yield of the reaction.



4.46 Mercury(II) halides can be converted into mercury(I) halides by combination with metallic mercury. Mercury(I) halides are known as mercurous halides. When chlorine is the halide, the resulting mercury salt is known as calomel:



When 2 grams of mercury(II) chloride reacts to produce 2 grams of calomel, calculate the percent yield of the reaction.

4.47 The Wurtz reaction results from the reaction of bromomethane (CH_3Br) with sodium to produce ethylene (C_2H_6)



How many grams of sodium are need to produce 3g of ethylene given that the yield of the reaction is 30%.

4.48 Nitriles with stannous chloride (SnCl_2) in the presence of hydrochloric acid produce an imine.



How many moles of imine (MW=43g/mol) are produced if we react 3g of nitrile (MW=41g/mol), with 2g of stannous chloride (MW=188g/mol) and 1g of hydrochloric acid (MW=36g/mol).

Ch. 5. Reactions in solution

THE most common reactions happen in solution and involve cations and anions. Think, for example, when you add sugar to your coffee or how metal rusts when it gets wet. The first example involves a dissolution reaction, whereas the second is a redox reaction in which electrons are exchanged. Overall there are three main different types of reactions happening in solutions. It is not only important to be able to differentiate these reactions, but it is also important to understand the nuances between acid-base reactions, precipitation reactions, and redox reactions. It is also critical to understand the properties of solutions and learn how to quantify and compare the amount of solute in a solution. On one hand, most of you will be surprised to know that water does not conduct electricity. This is because pure water is a weak electrolyte. On the other hand, the importance of electrolytes is well-known among the sports community. If you have ever played a sport, you have probably chugged a sports drink. These are electrolyte solutions. However, few know the specifics of their function. Electrolytes are salts that conduct electricity in water by separating them into positive and negative ions. To understand the properties of solutions it is important to identify and differentiate the different types of electrolytes.

5.1 Solutions and composition

Solutions are homogeneous mixtures of two components. The state of the matter of both components of the mixture or their polarity affects the formation of a solution. For example, a solution will not result from mixing oil and water as they have different polar characteristics and it will form from mixing table salt and water as both are polar chemicals. At the same time, the more solute you add to a solution the more concentrated the solution will be. This section covers polarity and the composition of solutions.

What makes a solution? Solutions are homogeneous mixtures of a solute and a solvent (see Figure 5.1). Homogeneous means that if you look at the mixture you will not be able to differentiate both components and you will only see it as a whole. In a solution, the solute is the component of the mixture in less amount, whereas the solvent is the component in a larger amount. Think about mixing sugar with water. Sugar is sweet and water tasteless. When you mix both, you form a solution of sugar (solute) in water (solvent) and you will not see sugar in the solution as it is dissolved. In this particular example, sugar will be the solute in the solution, as the sugar is in less amount than water. Is important to remember that a solution is a result of mixing a solute and a solvent:

$$\text{Solution} = \text{Solute} + \text{Solvent}$$



Sample Problem 45

Identify the solute and the solvent in the following mixtures: (a) 10g of H₂O(l) mixed with 3g of KCl(s); (b) 10g Cu(s) mixed with 3g Zn(s)

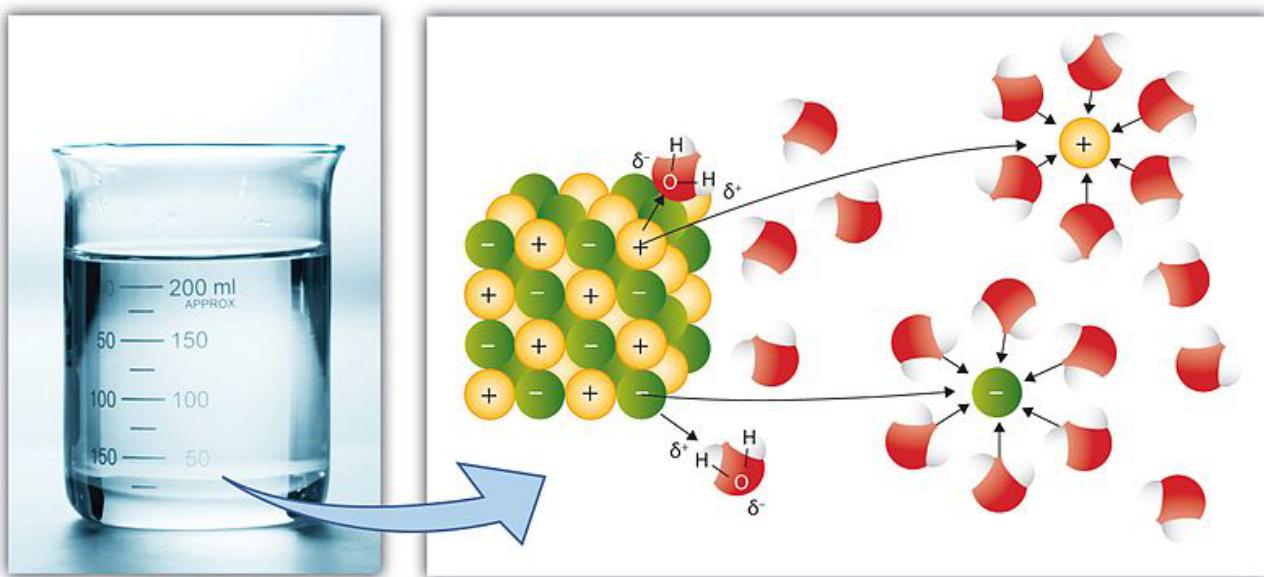
SOLUTION

(a) Potassium chloride is in less amount and hence will be the solute. Water, in larger quantity, will be the solvent. This is an example of an aqueous-based solution. (b) Zn is in less amount and hence will be the solute, and Cu the solvent. This is a solid solution.

◆ STUDY CHECK

Identify solute and solvent in the following mixture: (a) 10g of H₂O(l) and 20g of CH₃OH(l); (b) 1g of I₂(s) and 100g of CH₃CH₂OH(l)

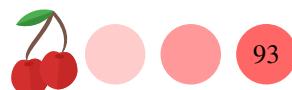
Types of solutions You can prepare different types of solutions by mixing a solid and a liquid, like when you mix sugar and water, or salt and water. You can create solutions as well by mixing two liquids or two solids. Examples are vinegar—a liquid solution of acetic acid (liquid) in water (liquid)—or steel— a solid solution that contains iron and carbon, both solids.



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Figure 5.1 A solution results from dissolving a solute into a solvent

Empirical rules of polarity The affinity between two chemicals is related to a concept called polarity. Molecules contain electrons and depending on the electron distribution within the molecules, molecules can be polar or non-polar. Molecules with an even electron distribution are non-polar as they have no permanent dipole moment. An example of this is H₂ molecule. Differently, HF is a polar molecule, as F concentrates more on the electron density of the molecule than H. The polar nature of substances—with a permanent dipole moment—is related to miscibility and molecules with similar polar character will mingle and mix creating a single visible phase (see Table ??). As an example, water (H₂O, polar) and methanol (CH₃OH, polar) will mix together. Differently, water (polar) and oil (non-polar) are immiscible due to their different polar nature and they will not mix. Even if the rules or polarity are based on



the nature and structure of the molecule, one can use very simple empirical rules to classify molecules as polar or non-polar. These rules work in general well for the case of diatomic and very large molecules:

- 1 **Rule one:** Diatomic molecules made of the same element (e.g. H₂) are non-polar.
- 2 **Rul two:** Diatomic molecules made of different elements (e.g. HI) are polar.
- 3 **Rul three:** Poliatomic molecules (with more than four atoms) made of C and H (e.g. CH₄) are in general non-polar.
- 4 **Rul four:** Poliatomic molecules (with more than four atoms) containing C, H, and a different atom (e.g. CH₃F) are in general polar.

Sample Problem 46

Classify the following molecules as polar or nonpolar: H₂, HCl, CH₃CH₃, and CH₃CH₂Cl.

SOLUTION

H₂ is a non-polar molecule, being a diatomic molecule containing two atoms of the same element. Differently HCl is polar. CH₃CH₃ is a non-polar poliatomic molecule made of C and H atoms, whereas CH₃CH₂Cl is polar.

◆ STUDY CHECK

Classify the following molecules as polar or nonpolar: HF, Cl₂, C₂H₄, and C₂H₃Cl.

Mixing and polarity A solution is formed when both the solute and the solvent mix. However, they will only mix if they have the same polarity. As an example, water (H₂O) is a polar molecule, and methanol (CH₃–OH) is too. Hence they will both mix and form a solution. If the elements of a mixture have different polarity they will not mix. An example is benzene (C₆H₆, nonpolar) and water, or for example oil (nonpolar) and water (polar).

Sample Problem 47

Use polarity arguments to indicate if the following substances will mix: (a) H₂O_(g) and CH_{4(g)}; (b) H₂O_(g) and HCl_(g)

SOLUTION

(a) Water and methane (CH₄) will not mix, as water is a polar molecule and CH₄ (methane) is nonpolar. (b) They will mix as HCl is a polar molecule and so is water.

◆ STUDY CHECK

Use polarity arguments to indicate if the following substances will mix: (a) H₂O_(l) and CH₃Cl_(l); (b) CH₃Cl_(l) and CCl_{4(l)}

Table 5.1 Polarity and mixing

Solvent	Solute	Mixing?
Polar	Polar	Yes
Polar	Nonpolar	No
Nonpolar	polar	No
Nonpolar	Nonpolar	Yes

5.2 Concentration of solutions

The concentration of a solution refers to the amount of solute with respect to the amount of solution. The larger concentration the larger the number of solute particles with respect to the particles of solvent. Concentration is one of the most important properties of a solution



as it affects the physical properties of a solution such as the freezing and boiling point. There are many different concentration units, such as molarity, mass percent concentration, or volume percent concentration. All these different units overall express the ratio between the particles—mass or volume—of solute and solvent.

Mass percent concentration The mass percent (% m/m) is the amount of solute in grams per gram of solution in percent form

$$\%m/m = \frac{\text{g of solute}}{\text{g of solution}} \times 100$$

Sample Problem 48

A NaCl solution is prepared by mixing 4g of NaCl with 50g of H₂O. Calculate the percent (m/m) of the solution.

SOLUTION

We need the grams of solute and the grams of solution. The grams of solute are given (4g of NaCl), whereas the grams of solution result from adding the grams of solvent and solute: 54 g of solution. Using the formula for the percent (m/m), we have:

$$m/m = \frac{4 \text{ g of solute}}{54 \text{ g of solution}} \times 100 = 7.4\%$$

This means that by mixing 4g of NaCl with 50g of H₂O you prepare a 7.4% (m/m) solution.

◆ STUDY CHECK

A KCl solution is prepared by mixing 5g of KCl with 200g of H₂O. Calculate the percent (m/m) of the solution.

Volume percent concentration The volume percent concentration (% v/v) is the volume of solute per volume of solution in percent form

$$\%v/v = \frac{\text{volume of solute}}{\text{volume of solution}} \times 100$$

Mass/volume percent concentration The mass/volume percent concentration (% m/v) is the mass of solute per mL of solution in percent form.

$$\%m/v = \frac{\text{g of solute}}{\text{mL of solution}} \times 100$$

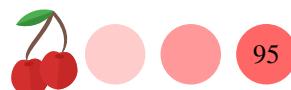
Molarity concentration The molarity (M) is the moles of solute per L of solution.

$$M = \frac{\text{moles of solute}}{\text{L of solution}}$$

Sample Problem 49

A NaCl solution is prepared by mixing 4g of NaCl (MW=58.4g/mol) with 50 g of water until a final volume of 52mL of solution. Calculate: (a) the mass percent (m/m) concentration; (b) the molarity.

SOLUTION



(a) to calculate the mass percent (m/m) we just need the grams of solute and the grams of solution—that is four plus fifty. Both numbers are already given:

$$m/m = \frac{\text{g of solute}}{\text{g of solution}} \times 100 = \frac{4 \text{ g of solute}}{54 \text{ g of solution}} \times 100 = 9.2\%$$

(b) To calculate molarity we need the moles of solute and the liters of solution. We have the mL of solution, that can be converted to L: $52\text{mL} = 5.2 \times 10^{-2}\text{L}$. To calculate the moles of solute, we will use the grams of solute and the molar mass to convert this value into moles: $4\text{g}/58.4\text{g/mol} = 0.068\text{moles}$. Plugging all values into the molarity formula:

$$M = \frac{\text{moles of solute}}{\text{L of solution}} = \frac{0.068 \text{ moles of solute}}{5.2 \times 10^{-2}\text{L of solution}} = 1.31M$$

◆ STUDY CHECK

(a) A solution is prepared by mixing 8g of NaCl (MW=74g/mol) with 250mL of H₂O. Calculate the molarity; (b) A KCl solution is prepared by mixing 45g of KCl with 200g of H₂O. Calculate the percent (m/m) of the solution.

Concentration units as conversion factors Each of the different concentration units—molarity, mass percent, volume percent, mass/volume percent—can be used in a conversion factor form. For example, if the molarity of a solution is 3M, this means that in the solution there are 3 moles of solute in every liter of solution.

3M	or	$\frac{3 \text{ mol of solute}}{1 \text{ L of solution}}$	or	$\frac{1 \text{ L of solution}}{3 \text{ mol of solute}}$
----	----	---	----	---

Similarly, if the mass percent of a solution is 5% this means that there are 5 grams of solute for every 100 grams of solution. We often use concentration units as conversion factors when we need to transform between one unit on top (bottom) of the conversion factor and the unit on the bottom (top).

Sample Problem 50

How much volume of a 4M solution do you need to provide 5 moles of solute.

SOLUTION

We will use the conversion factor of Molarity using the volume on top and the moles on the bottom in order to cancel the units:

$$\frac{5 \text{ moles of solute}}{4 \text{ moles of solute}} \times \frac{1 \text{ L of solution}}{} = 1.25\text{L}$$

This means that 1.25L of a 4M solution will provide 5 moles of solute.

◆ STUDY CHECK

How many grams of a 6% (m/m) solution do you need to provide 5 grams of solute.

Molarity calculation involving grams As molarity is just the ratio between the moles of solute and the liters of the solution, we can use this property to calculate the mass of solute contained in a certain volume of solution. We will proceed by first calculating the number of moles in that volume to then convert moles into grams.



5.3 Dilution

Dilution is the process of preparing a diluted solution from a more concentrated solution. Solutions are often stored in a stock room in concentrated form. These stocks should be diluted before use. To dilute a solution we need to take a certain amount of the concentrated solution and add water. When adding water, the number of moles of solute does not change, and the concentration always decreases. We have a concentrated solution (c_1) and we need to prepare a certain volume (V_2) of a more diluted solution (c_2). The question is how much volume of the concentrated solution (V_1) we need to take. To answer this we should use the following formula:

$$c_1 \cdot V_1 = c_2 \cdot V_2$$

Sample Problem 51

How many liters of a 3M NaCl solution are required to prepare 2L of a 1M diluted NaCl solution.

SOLUTION

We have a concentrated solution of 3M molarity and we want to prepare a more dilute solution. In particular 2L of a 1M. Hence: $c_1 = 3$ and $c_2 = 1M$ and $V_2 = 2L$. Using the dilution formula:

$$3M \cdot V_1 = 1M \cdot 2L$$

Solving for V_1 we have a volume of 0.66L.

❖ STUDY CHECK

How many liters of a 5M NaCl solution are required to prepare 3L of a 3M diluted NaCl solution.

5.4 Electrolytes and insoluble compounds

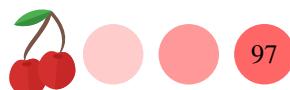
On one hand, electrolytes are compounds that conduct electricity once dissolved in water. Differently, nonelectrolytes are compounds that do not conduct electricity once dissolved in water. On the other hand, insoluble compounds are not soluble in water, whereas soluble compounds can be dissolved in water. This section covers the properties of electrolytes and insoluble (and soluble) compounds. At the end of this section, you should be able to classify a chemical in terms of its electrolyte type and solubility character.

Solubility formula Solubility (s) is the grams of a solute per 100 g of solvent:

$$s = \frac{\text{g of solute}}{100 \text{ g of solvent}}$$

A saturated solution can be achieved when you fit the maximum amount of solute in the solvent. If you continue adding solute to a saturated solution it will precipitate and a solid will form.

Soluble and insoluble salts Soluble compounds dissolve in water, whereas insoluble compounds do not. For example, barium chromate ($\text{BaCrO}_4(s)$) is an insoluble salt. How do we know that? Table 5.2 will help you predict the solubility of a salt. To



do this, you need to start by assessing the right ion (the anion, CrO_4^{2-}) located in the left column of Table 5.2. After that, you need to assess the left ion (the cation, Ba^{2+}) located in the right column. If you follow this, you will see that chromate is insoluble and barium is not part of any exception. Let us predict for example the soluble/insoluble nature of CaSO_4 , calcium sulfate. We start by looking for SO_4^{2-} in the left column to find out it is soluble. Next, we continue in the same line as SO_4^{2-} and look for the ion in the left Ca^{2+} . In conclusion, even when SO_4^{2-} is soluble, when combined with Ca^{2+} , we have that CaSO_4 is insoluble, and overall $\text{CaSO}_4(s)$ is insoluble.

Sample Problem 52

Predict the soluble/insoluble nature of the following compounds: (a) K_2CO_3 , (b) NaNO_3 and (c) $\text{Ca}(\text{OH})_2$.

SOLUTION

(a) $\text{K}_2\text{CO}_3(aq)$ is soluble, as CO_3^{2-} is insoluble but when combined with K^+ the salt becomes soluble. (b) All nitrates are soluble without exceptions. (c) $\text{Ca}(\text{OH})_2(aq)$ is soluble.

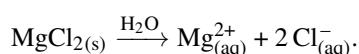
◆ STUDY CHECK

Predict the soluble/insoluble nature of the following compounds: (a) Li_3PO_4 (b) Na_2S (c) AgCl

Table 5.2 Soluble and insoluble compounds

Ions that form <i>soluble</i> compounds...	... except when combined with
Group I ions (Na^+ , Li^+ , K^+ , etc)	no exceptions
Ammonium (NH_4^+)	no exceptions
Nitrate (NO_3^-)	no exceptions
Acetate (CH_3COO^-)	no exceptions
Hydrogen carbonate (HCO_3^-)	no exceptions
Chlorate (ClO_3^-)	no exceptions
Halide (F^- , Cl^- , Br^- , I^-)	Pb^{2+} , Ag^+ and Hg_2^{2+}
Sulfate (SO_4^{2-})	Ag^+ , Ca^{2+} , Sr^{2+} , Ba^{2+} , Hg_2^{2+} and Pb^{2+}
Ions that form <i>insoluble</i> compounds...	... except when combined with
Carbonates (CO_3^{2-})	group I ions (Na^+ , Li^+ , K^+ , etc) or ammonium (NH_4^+)
Chromates (CrO_4^{2-})	group I ions (Na^+ , Li^+ , K^+ , etc) or Ca^{2+} , Mg^{2+} or ammonium (NH_4^+)
Phosphates (PO_4^{3-})	group I ions (Na^+ , Li^+ , K^+ , etc) or ammonium (NH_4^+)
Sulfides (S^{2-})	group I ions (Na^+ , Li^+ , K^+ , etc) or ammonium (NH_4^+)
Hydroxides (OH^-)	group I ions (Na^+ , Li^+ , K^+ , etc) or Ca^{2+} , Mg^{2+} , Sr^{2+} or ammonium (NH_4^+)

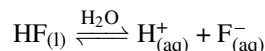
Strong electrolytes Strong electrolytes completely dissociate in water. Hence, in a solution of a strong electrolyte, you will only have ions and never molecules. Strong electrolytes are typically ionic compounds such as MgCl_2 or NaCl (table salt). We represent the dissociation of a strong electrolyte with a single arrow, meaning that the reaction proceeds to completion, and for the example below, in the solution, we will only have ions ($\text{Mg}_{(aq)}^{2+} + 2 \text{Cl}_{(aq)}^-$) and not molecules ($\text{MgCl}_{2(s)}$):



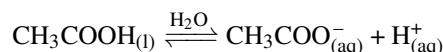
Weak electrolytes Weak electrolytes partially dissociate in water, and this is indicated using a chemical reaction with a double arrow. Hence in a solution of a weak electrolyte, you will have ions as well as molecules at the same time. Examples of weak



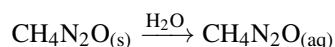
electrolytes are hydrofluoric acid, water, ammonia, or acetic acid. The dissociation of hydrochloric acid (HF) proceeds as:



Acetic acid (CH_3COOH) is an important weak electrolyte and its dissociation proceeds somehow in a peculiar way:



Nonelectrolytes Nonelectrolytes do not dissociate in water. Hence a solution of a nonelectrolyte will only contain molecules and not ions. Examples of nonelectrolytes are carbon-based chemicals such as methanol, ethanol, urea, or sucrose. The dissociation of urea for example $\text{CH}_4\text{N}_2\text{O}$ proceeds as:



Identify the electrolyte character of a chemical You can use Table 5.3 to identify the electrolyte character of a chemical. Ionic compounds are in general strong electrolytes, and most acids are as well. There are four important weak electrolytes: water, acetic acid, ammonia, and hydrofluoric acid. Covalent compounds are in general nonelectrolytes. Organic compounds, compounds based on carbon atoms (e.g. $\text{C}_{12}\text{H}_{22}\text{O}_{11}$) are in general nonelectrolytes.

Table 5.3 Different types of electrolytes

Electrolyte Type	Dissociation	Particles in solution	Examples
Strong	Fully	Mostly ions	Ionic Compounds and most acids and bases (hydroxides): NaCl , NaOH , HCl , MgCl_2 , H_2SO_4 , etc
Weak	Partially	Ions & molecules	NH_3 , CH_3COOH (acetic acid), HF , H_2O
Nonelectrolytes	No	molecules	Most covalent compounds: CH_3OH (methanol), $\text{CH}_3\text{CH}_2\text{OH}$ (ethanol), $\text{C}_{12}\text{H}_{22}\text{O}_{11}$ (sucrose), CH_4NO_2 (urea)

Sample Problem 53

For the following chemicals indicate whether you will have in the solution (a) only ions, (b) ions and some molecules, or (c) molecules: NH_3 , KOH , and $\text{C}_{12}\text{H}_{22}\text{O}_{11}$.

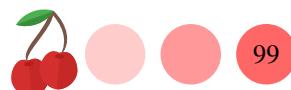
SOLUTION

Ammonia (NH_3) is a weak electrolyte and a solution of ammonia will contain ions and well as ammonia molecules. Differently KOH is a strong electrolyte and in solution you would find only ions (K^+ and OH^-). Sucrose ($\text{C}_{12}\text{H}_{22}\text{O}_{11}$) is a nonelectrolyte and in solution you will find molecules.

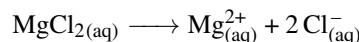
❖ STUDY CHECK

For the following chemicals indicate whether you will have in the solution only ions, ions and some molecules, or molecules: (a) H_2SO_4 , HNO_3 and CH_3OH .

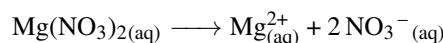
Breaking down electrolytes into ions Electrolytes—in particular strong electrolytes—dissociate producing ions. This way, a solution of for example NaCl does not contain NaCl molecules but $\text{Na}_{(\text{aq})}^+$ cations and $\text{Cl}_{(\text{aq})}^-$ anions. Hence it is important to correctly break down electrolytes into ions. To do this, you need to revert the



combination of ions that produce a given chemical while making sure the charges are balanced. For example, let us break magnesium chloride $MgCl_{2(aq)}$ into ions. This is a strong electrolyte formed by magnesium cations and chloride anions. The valence of magnesium is +II and the valence of chlorine is -I. The $MgCl_2$ formula also tells us we have one magnesium and two chlorines. The overall process is:



Another example, magnesium nitrate $Mg(NO_3)_2$. This strong electrolyte—as this is an ionic salt—is made of magnesium with valence +II and nitrate with valence -I. The formula indicates we have one $Mg_{(aq)}^{2+}$ and two $NO_3^-_{(aq)}$. Hence:



Sample Problem 54

Break down the following chemicals into ions, if possible:

Chemical	Particles in solution
$K_2CrO_4(aq)$	
$Ba(NO_3)_2(aq)$	
$BaCrO_4(s)$	
$KNO_3(aq)$	

SOLUTION

We can only break down into ions ionic compounds and oxosalts that are not solid. From the list of chemicals in the example, we will not be able to break down $BaCrO_4(s)$ into ions as it is a solid. From the other chemicals, $K_2CrO_4(aq)$ is named potassium chromate and contains $2K_{(aq)}^+$ and $CrO_4^{2-}_{(aq)}$ ions. Barium nitrate— $Ba(NO_3)_2(aq)$ —will produce $Ba_{(aq)}^{2+}$ and $2NO_3^-_{(aq)}$. Finally, potassium nitrate— $KNO_3(aq)$ —will produce $K_{(aq)}^+$ and $NO_3^-_{(aq)}$. In the table:

Chemical	Particles in solution
$K_2CrO_4(aq)$	$2K_{(aq)}^+$ + $CrO_4^{2-}_{(aq)}$
$Ba(NO_3)_2(aq)$	$Ba_{(aq)}^{2+}$ + $2NO_3^-_{(aq)}$
$BaCrO_4(s)$	$BaCrO_4(s)$
$KNO_3(aq)$	$K_{(aq)}^+$ + $NO_3^-_{(aq)}$

◆ STUDY CHECK

Break down the following chemicals into ions, if possible: $H_2O(l)$, $NH_3(l)$, $AgNO_3(aq)$.

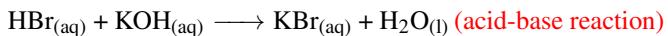
5.5 An introduction to reactions in solution

There are three different reactions in solution: acid-base reactions, precipitation reactions, and redox reactions. The key to identifying acid-base reactions is in the reactants, as an acid-base reaction results from the reaction between an acid and a base. Precipitation reactions



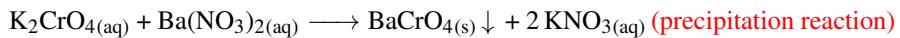
are reactions that produce a precipitate. Hence, the key to identifying a precipitation reaction is in the products. Precipitation reactions always contain a solid as a product. Redox reactions contain two elements with different redox numbers in the reactants and products. The key to identifying redox reactions is to be able to spot elements with different oxidation states, for example: Cu and Cu²⁺ or H⁺ and H₂. In the following, we will describe more about the three different types of reactions in solution. The goal of this section is for you to be able to identify each type.

Acid-base reactions Acid-base reactions result from the reaction of an acid with a base. Both produce water and another chemical. An example is:



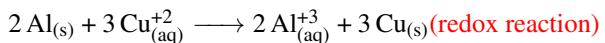
Hydrobromic acid (HBr) is an acid and potassium hydroxide (KOH) is a base. The result of an acid-base reaction is always water and an ionic compound, in this case KBr.

Precipitation reactions Precipitation reactions result in an insoluble chemical, that is, results in a solid chemical. An example would be:



The chemical BaCrO_{4(s)} is a solid that precipitates in the solution, hence the name of the type of reaction. The symbol on BaCrO_{4(s)} ↓ represents the precipitation process. The solubility of a given solute such as BaCrO_{4(s)} is the amount of solute (in grams) that can be dissolved in a given mass of solvent (in particular 100 g of solvent). A solute with a low solubility will be hard to dissolve. Think about cacao and water. The solubility of cacao is low and hence by simply adding cacao powder to water, you will not be able to make a solution. However, solubility depends on the solute and solvent combination, but also on the temperature, and by warming up a solvent you can increase solubility and fit more solute in the same amount of solvent. This section covers different aspects of solubility.

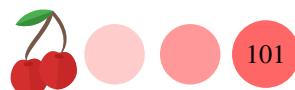
Redox reactions Redox reactions are different than acid-base or precipitation reactions. They contain the same chemical element in two different states resulting from the loss or win of electrons. Look for the example:



We have that neither Al_(s) or Cu_(aq)⁺² are an acid or a base, therefore this is not an acid-base reaction. Also, there is no insoluble product, hence this is not a precipitation reaction. Indeed, this is a redox reaction, as we have Al in two different states: as metallic Al_(s) and as ionic Al_(aq)⁺³, which result from the loss of three electrons. Therefore in a redox reaction, there are always elements in the chemicals that lose electrons. In redox reactions, there is also an element that wins electrons. For example, Cu_(s) and Cu_(aq)⁺² have different redox number. In particular, Cu_(aq)⁺² is the result of removing three electrons from Cu_(s). At this point, we have that this reaction is redox as it contains an element that gains electrons and an element that loses electrons. Sometimes, the redox state of the elements is not that obvious. Look at this example:



This is a redox reaction as you can find iron and copper in two states, metallic and also ionic. Therefore, these two metals have two different redox numbers in the reaction.

**Sample Problem 55**

Classify the following reactions as acid-base, redox or precipitation.

- $\text{Fe}_{(s)} + \text{Cu}_{(aq)}^{+2} \longrightarrow \text{Fe}_{(aq)}^{+2} + \text{Cu}_{(s)}$
- $\text{AgNO}_{3(aq)} + \text{NaCl}_{(aq)} \longrightarrow \text{AgCl}_{(s)} + \text{NaNO}_{3(aq)}$
- $2 \text{HCl}_{(aq)} + \text{Ca(OH)}_2{}_{(aq)} \longrightarrow \text{CaCl}_{2(aq)} + 2 \text{H}_2\text{O}_{(l)}$

SOLUTION

The first reaction is a redox reaction. This is because we can find two different oxidation states for Cu and also for Fe. That means one of these elements lost electrons and the other won electrons. The second reaction is a precipitation reaction as it produces a solid. The last reaction is an acid base, as the reactants are an acid and a base.

◆ STUDY CHECK

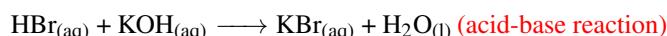
Classify the following reactions as acid-base, redox or precipitation.

- $\text{HNO}_{2(aq)} + \text{NaOH}_{(aq)} \longrightarrow \text{NaNO}_{2(aq)} + \text{H}_2\text{O}_{(l)}$
- $2 \text{Na}_{(s)} + \text{Cl}_{2(g)} \longrightarrow 2 \text{NaCl}_{(s)}$
- $\text{MgCl}_{2(aq)} + 2 \text{AgNO}_{3(aq)} \longrightarrow 2 \text{AgCl}_{(s)} + \text{Mg(NO}_3)_2{}_{(aq)}$

5.6 Precipitation reactions and acid-base reactions

This section deals with two important types of reactions in solution. Precipitation reactions are characterized by the products and acid-base by the reactants. In an acid-base reaction, the reactants are an acid and a base, and they react to produce water and another chemical. Precipitation reactions produce a precipitate, that is, a solid.

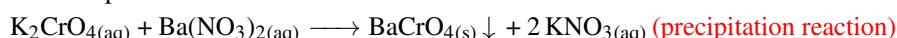
Acid–base reactions Acid-base reactions result from the reaction of an acid with a base. Both produce water and another chemical. An example is:



Hydrobromic acid $\text{HBr}_{(aq)}$ is an acid and potassium hydroxide is a base.

Precipitation reactions Precipitation reactions result in an insoluble chemical.

An example would be:



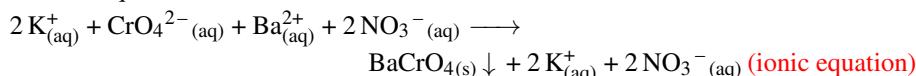
The chemical $\text{BaCrO}_{4(s)}$ is a solid that precipitates in the solution. The solubility of a given solute such as $\text{BaCrO}_{4(s)}$ is the amount of solute (in grams) that can be dissolved in a given mass of solvent (in particular 100 g of solvent). A solute with a low solubility will be hard to dissolve. Think about cacao and water. The solubility of cacao is low and hence by simply adding cacao powder to water, you will not be able to make a solution. However, solubility depends on the solute and solvent combination, but also on the temperature, and by warming up a solvent you can increase solubility and fit more solute in the same amount of solvent. This section covers different aspects of solubility.

Formula equations, ionic equations and net ionic equations

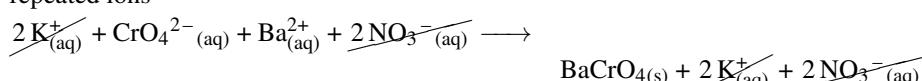
Electrolytes in solutions contain ions—cations and anions—however when we write chemical formulas we barely show those ions. Differently, we just write the formulas and that is the reason that chemical equations are referred to as *formula equation*. Look for the example:



In this equation, $\text{K}_2\text{CrO}_4(\text{aq})$ is actually in the form of ions: $2\text{K}^+(\text{aq})$ and $\text{CrO}_4^{2-}(\text{aq})$. At the same time, $\text{Ba}(\text{NO}_3)_2(\text{aq})$ in the form of ions results in $\text{Ba}^{2+}(\text{aq})$ and $2\text{NO}_3^-(\text{aq})$. Also, $2\text{KNO}_3(\text{aq})$ contains $2\text{K}^+(\text{aq})$ and $2\text{NO}_3^-(\text{aq})$. Finally, $\text{Ba}(\text{CrO}_4)(\text{s})$ does not produce any ions in the solution, as it is solid. Ionic equations result from writing all ions in a formula equation:



However, the ionic equation contains repeated ions. Look for example the previous equation with $2\text{K}^+(\text{aq})$ on the left and the right of the equation. If we simplify the repeated ions



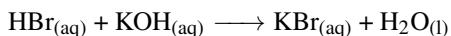
we obtain what is called as the *net ionic equation*:



Overall, we have that the formula equation, ionic equation, and net ionic equation are just three different ways to express the same chemical equation. The first form includes only molecules whereas the second included all ions produced by each chemical. The last form includes only ions that are not repeated on both sides of the equation.

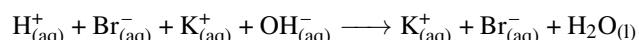
Sample Problem 56

Write down the ionic equation and net ionic for the following formula equation:

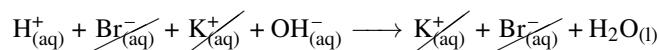


SOLUTION

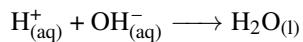
Mind we can only break down strong electrolytes. Hence, water will not be expressed in the form or ions as it is a weak electrolyte. If we break down the other chemicals we have the ionic equation:



If we eliminate the ions that are repeated in both sides:

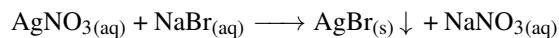


we have the net ionic equation:



❖ STUDY CHECK

Write down the ionic equation and net ionic for the following formula equation:

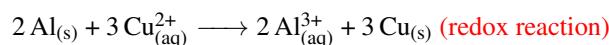


5.7 Redox reactions

Redox reactions are different than acid-base or precipitation reactions. They contain the same chemical element in two different states resulting from the loss or win of electrons.



For example:



We have that neither $\text{Al}_{(\text{s})}$ or $\text{Cu}_{(\text{aq})}^{2+}$ are an acid or a base. Also, there is no product precipitate. Hence, this reaction is not an acid-base reaction or a precipitation reaction. This is a redox reaction, as we have Al in two different states: as metallic $\text{Al}_{(\text{s})}$ and as ionic $\text{Al}_{(\text{aq})}^{3+}$, which result from the loss of an electron. In redox reaction, there is always elements in the chemicals that lose electrons and chemicals winning electrons.

Oxidation state or redox number The redox number also called oxidation number or oxidation state helps compare elements that have lost (or gained) different charges. When comparing two elements with different redox numbers, the larger this number the more electrons the element has lost. Similarly, the smaller this number the more electrons the element has won.

Rules to calculate redox numbers We indicate redox numbers with a roman number on top of the element. For example, the redox number of manganese in this compound is +7: $\text{Mn}^{\text{VII}}\text{O}_4^-$. The redox number can be noninteger. There are five rules to identify the redox number of an element.

- ¶ **Rule 1** Single atoms or elements have zero redox number. Examples are Na or H_2 , both with redox zero.
- ¶ **Rule 2** Monoatomic ions have redox number equal to their charge. Examples are Na^+ or Cl^- with redox +1 and -1, respectively.
- ¶ **Rule 3** The redox number of fluorine is -1
- ¶ **Rule 4** The redox number of hydrogen on its covalent (e.g. H_2O) compounds is +1.
- ¶ **Rule 5** The redox number of oxygen in normal oxides (e.g. MgO) is normally -2, with the exception of peroxides (e.g. H_2O_2) in which is -1.

Calculating the redox number How do we calculate the redox number for example of manganese in this chemical: MnO_4^- , permanganate? To do this, we need to set up a formula so that the redox numbers of all elements in the molecule—taking into account the number of atoms in the molecule—are equal to the charge. In the case of permanganate, let us call x to the redox number of manganese. We know the redox of oxygen is -2 and we have four oxygens in the molecule. We also know the charge of the ion is -1. Therefore we have:

$$x + 4 \cdot (-2) = -1$$

If we solve for x we obtain the redox number of manganese of VII.

Sample Problem 57

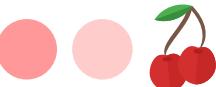
Calculate the redox number of the elements underlined in the following molecules: (a) K_2CO_3 and (b) H_2CO .

SOLUTION

Let us set up the redox equation for the first compound, knowing that the redox of oxygen is -2 and potassium +1. The unknown variable x represents the redox number of the underlined element. We have:

$$2 \cdot (+1) + x + 3 \cdot (-2) = 0$$

Mind we have two potassium and three oxygens hence we need to time the



redox of K by two and the redox of O by three. If we solve for x we obtain a redox number for carbon of IV. The redox equation for the second example is:

$$2 \cdot (+1) + x + (-2) = 0$$

Mind that according to the redox rules, the redox number of oxygen is +1. Solving for x we have a redox number of zero.

STUDY CHECK

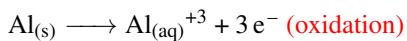
Calculate the redox number of the elements underlined in the following molecules: (a) Cr₂O₇²⁻ and (b) Cr₂O₃

Redox means oxidation and reduction By comparing the redox number of the same element in two different compounds we can figure out in what compound the element has lost or gained electrons. Look for example the case of Cr^{VI}₂O₇²⁻ and Cr^{III}₂O₃. The same element in two different molecules has two different redox numbers. In the case of dichromate, the redox of Cr is VI, whereas in the case of chromium(III) oxide the redox of Cr is III. The larger the redox number the more oxidized is the element, and that means the element has lost electrons. The smaller the redox number the more reduced the element and that means it has gained electrons. If we compare both cases, we have that Cr in dichromate is oxidized—it lost electrons—and Cr in chromium(III) oxide is reduced—it gained electrons.

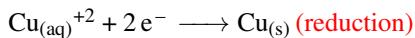
Redox numbers in chemical reactions The goal is to identify the element that undergoes oxidation and reduction in a chemical reaction. We can reach this goal by using the half-reaction method. Every redox reaction is composed of two processes, reduction, and oxidation. These two processes can be separated into two half-reactions so that the combination of both half-reactions leads to a balanced redox. Let us work on a simple unbalanced redox reaction:



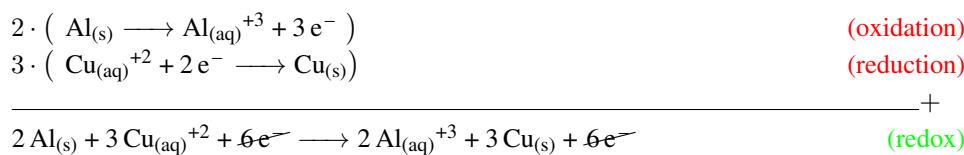
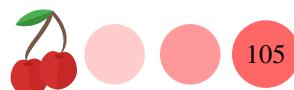
Solid Al_(s) on the reactant side has zero redox number, whereas ionic Al_(aq)⁺³ on the product side has a redox number equal to III. Al has undergone oxidation as its redox number increases from zero to three. Al has lost three electrons. We can write the oxidation half-reaction:



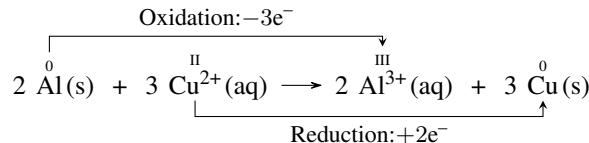
Mind that electrons have a negative charge and we add electrons to compensate for the charge of Al_(aq)⁺³. Now let us compare the redox number of Cu. In the reactant side we have Cu_(aq)⁺² with redox of II. On the product side, we have Cu_(s) with zero redox number. Cu has undergone reduction as its redox number has decreased. This means it has gained electrons, in particular, two electrons:



Balancing simple redox reactions The goal here is to balance a redox chemical reaction by combining two half-reactions. In the example above the oxidation and reduction involving a different number of electrons. Hence to be able to add both redox we need to time each half-reaction by a number so that the number of electrons cancels out. As the first reaction involved three electrons and the second two, we will do:

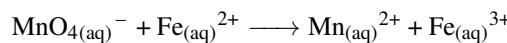


The overall balanced redox equation is:

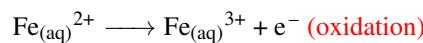


5.8 Redox in acidic and basic medium

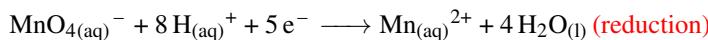
Balancing redox reactions in acidic medium Redox reactions happen in either basic or acidic medium. Here we will go over how to balance redox reactions in acidic medium. In order to do this we will first separate the reaction in two half-reactions. In each semi-reaction we will balance all elements but hydrogen and oxygen. When all elements are balanced, we will proceed to balance O by adding H₂O molecules and we will balance H by adding H⁺. Finally, we will add electrons to compensate the charge of the reaction. Let us work on an example:



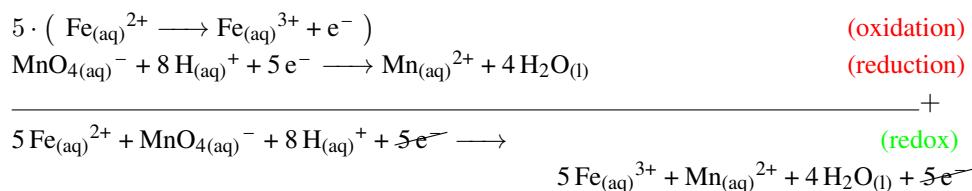
One of the semi-reactions involve Manganese whereas the other involves Iron. The redox number of Mn in permanganate is VII hence Manganese is being reduced, as its redox number decreases from VII to II, whereas Iron is being oxidized as its redox number increases from II to III. The oxidation half-reaction does not contain hydrogen or oxygen hence we will only have to balance the charger with one electron:

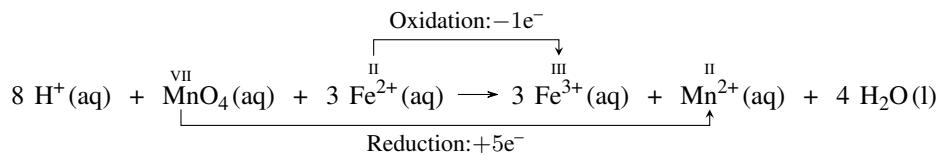


The reduction half-reaction contains oxygen. Hence, we will have to add H₂O molecules to balance oxygen and H⁺ to balance hydrogen. In particular, we will need two water molecules—as MnO₄⁻ has four oxygens and we will have to add eight protons as we are adding four molecules of water. Finally, we need to add three electrons to equalize the charge:



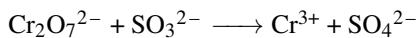
As the oxidation involves one electron and the reduction three, we need to time the oxidation by three:





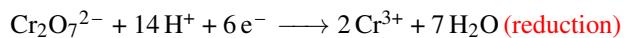
Sample Problem 58

Balance the following redox in acidic medium:

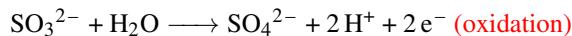


SOLUTION

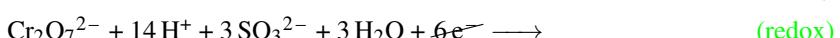
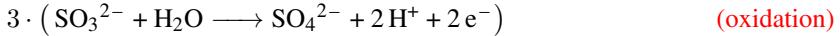
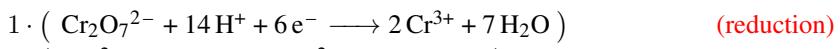
We locate the same element in both sides of the reaction with different redox number. We found Chromium in the form of dichromate ($\text{Cr}_2\text{O}_7^{2-}$) with redox number VI and Chromium in the product side with redox III. Therefore Chromium is being reduced, as its redox number decreases. Differently, we found sulphur in the reactants side in the form of sulfite (SO_3^{2-}) with redox number of IV and in the product side with redox number of VI. Therefore Sulphur is being oxidized. We will first set up the oxidation half-reaction knowing that we have different amounts of Cr in both side and that we will have to add water molecules to balance O and protons to balance H. As we have seven oxygens in $\text{Cr}_2\text{O}_7^{2-}$ we will have to add seven water molecules. Also, as we add seven water molecules we will have to add fourteen protons. We will need six electrons to compensate the charge:



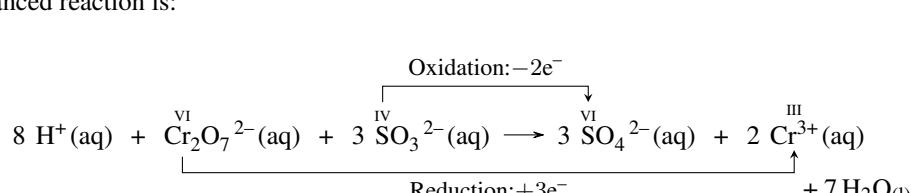
For the reduction half-reaction, we have a difference of one oxygen atoms and hence we will need one water molecule and two protons; we will need two electrons to compensate the charge:



In order to add both half-reactions as the reduction involves two electrons and the oxidation six, we will have to multiply the reduction half-reaction by three:

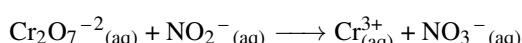


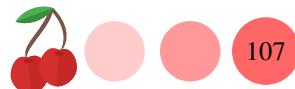
After we cancel the electrons and eliminate protons and water molecules, the balanced reaction is:



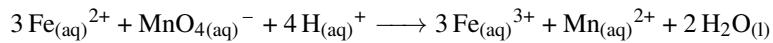
❖ STUDY CHECK

Balance the following redox in acidic medium:

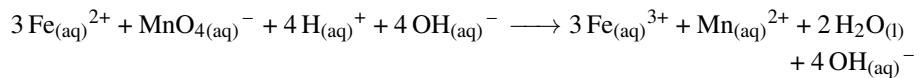




Balancing redox reactions in basic medium To balance a redox in a basic medium we need first to balance the reaction in an acidic medium. After, we will compensate all H⁺ with OH⁻ in both sides of the reaction. Mind that when combining H⁺ with OH⁻ we obtain H₂O. For example, to balance the following reaction in a basic medium:



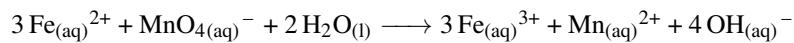
we will add four OH⁻ in both sides:

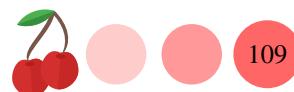


And after canceling the four protons with the four hydroxyls, we have:



Now we have four water molecules in the left and two in the right. We will cancel two molecules from each side in order not to report water molecules twice:





CHAPTER 5

SOLUTIONS

5.1 A solution is prepared by mixing 4 g of $C_6H_{14(l)}$ and 10 g of $CCl_{4(l)}$. Indicate the true statement: (a) C_6H_6 is the solute (b) CCl_4 is the solute (c) Both chemicals do not mix (d) The mixture is not a solution

5.2 A solution is prepared by mixing 5 g of $Au_{(s)}$ and 2 g of $Cu_{(s)}$. Indicate the true statement: (a) Au is the solute (b) Cu is the solute (c) Both elements do not mix (d) The mixture is not a solution

5.3 Classify the following molecules as polar or nonpolar: (a) $C_6H_{14(l)}$ (b) $CH_3CH_2CH_2OH_{(l)}$ (c) $C_5H_{10(l)}$ (d) $C_6H_5CH_3_{(l)}$ (e) $CH_3CH_2OH_{(l)}$ (f) $C_6H_5NH_2_{(l)}$

5.4 Classify the following molecules as polar or nonpolar: (a) $H_2O_{(l)}$ (b) $C_5H_{12(l)}$ (c) $CH_3COOH_{(l)}$ (d) $CH_3OH_{(l)}$

5.5 Which chemicals from the following list will mix with $H_2O_{(l)}$: (a) $NH_3_{(l)}$ (b) $C_5H_{12(l)}$ (c) $C_6H_{14(l)}$

5.6 Which chemicals from the following list will mix with $C_5H_{12(l)}$: (a) $H_2O_{(l)}$ (b) $C_6H_{14(l)}$ (c) $CH_3COOH_{(l)}$

ELECTROLYTES AND INSOLUBLE COMPOUNDS

5.7 Break down the following compounds into ions: (a) $Ca(OH)_2$ (b) K_2CrO_4 (c) $Ca(NO_3)_2$

5.8 Break down the following compounds into ions: (a) H_2SO_4 (b) HNO_3 (c) $KMnO_4$

5.9 Indicate whether solutions of the following chemicals will have ions (I), ions and molecules (I+M), or just molecules (M):

Chemical	I	I+M	M
NaCl			
HCl			
CaCl ₂			

5.10 Indicate whether solutions of the following chemicals will have ions (I), ions and molecules (I+M), or just molecules (M):

Chemical	I	I+M	M
H_2O			
NO_2			
CO_2			

5.11 Indicate the soluble/insoluble character of the following compounds:

Chemical	Soluble	Insoluble
$AgNO_3$		
$AgBr$		
$CaCO_3$		
Na_2CO_3		

5.12 Indicate the soluble/insoluble character of the following compounds:

Chemical	Soluble	Insoluble
$NaCH_3COO$		
$NaHCO_3$		
Ag_2SO_4		
$NaCrO_4$		
CaS		

CONCENTRATION UNITS

5.13 Order the following solution from more to less concentrated: (a) A vanillin solution ($1.3 \times 10^{-1} M$) (b) An adrenaline solution ($1.1 \times 10^3 M$) (c) Vinegar, an acetic acid solution ($1.2 \times 10^0 M$)

5.14 Order the following solution from more to less concentrated: (a) Solution A ($4.3 \times 10^{-5} M$) (b) Solution B ($6.1 \times 10^{-3} M$) (c) Solution C ($6.4 \times 10^{-4} M$)

5.15 Sodium hydroxide $NaOH$, a very strong base, is a chemical used in drain cleaners. A drain cleaning solution is prepared by mixing 25g of $NaOH$ in 250g of water. Calculate the mass percent of solute.



5.16 A solution is prepared by mixing 15g of KCl in 50g of water. Calculate the mass percent of solute.

5.17 Alcohol-hydroxide is a mixture of a base with an organic alcohol, employed to clean glass. An alcohol-hydroxide mixture is prepared by mixing 60g of NaOH with 500g of ethanol. Calculate: (a) the mass percent of solvent. (b) the mass percent of solute.

5.18 Vinegar is not a pure chemical, it is indeed a (m/m) 5% acetic acid solution. How many grams of acetic acid are there in 2g of vinegar.

5.19 Vanilla extract is a solution vanillin in ethanol. A vanilla solution is made by mixing 15 mL of pure vanillin and 50mL of ethanol. Calculate the Percent Volume/Volume.

5.20 A solution is made by mixing 2 mL of a solute and 100mL of solvent. Calculate the Percent Volume/Volume.

5.21 An HCl solution is prepared by mixing 4 moles of HCl with water until reaching a volume of 250mL. Calculate the molarity of the solution.

5.22 How many mL of a 3M KCl solution contains 0.06 moles of KCl.

5.23 How many mL of a 4M NaCl (MW=58g/mol) solution contains 5 grams of NaCl.

5.24 How many mL of a 1M NaCl (MW=58g/mol) solution contains 4 grams of NaCl.

5.25 How many grams of solute are there in 100mL of a 0.01M HNO₃ (MW=63g/mol) solution.

5.26 How many mL of a 0.001M Ca(OH)₂ (MW=74g/mol) solution can be prepared from 5 mg of Ca(OH)₂.

5.27 What is the final volume when 50mL of a 2M NaCl solution is diluted to a 1M.

5.28 What is the concentration of a solution prepared when 100mL a 4% HCl solution is diluted to a final vol-

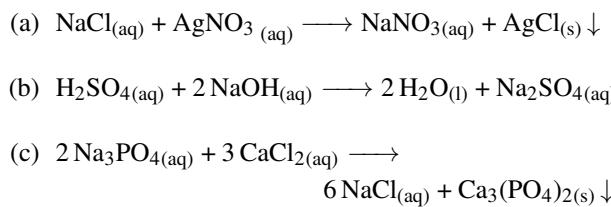
ume of 500mL.

5.29 Describe how to prepare 50mL of a 0.5M H₂SO₄ solution, starting with a 1M stock H₂SO₄ solution.

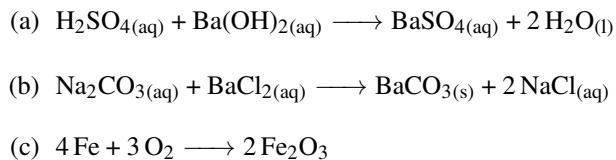
5.30 Describe how to prepare 100mL of a 0.1M H₂SO₄ solution, starting with a 2M stock H₂SO₄ solution.

PRECIPITATION AND ACID-BASE REACTIONS

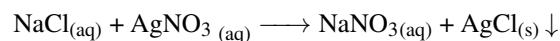
5.31 Classify the following reaction as acid-base, precipitation, or redox:



5.32 Classify the following reaction as acid-base, precipitation, or redox:



5.33 Obtain the net ionic equation for the following reaction:

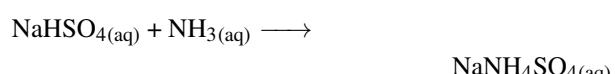


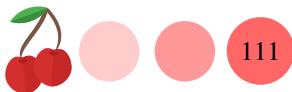
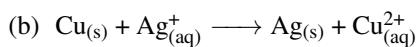
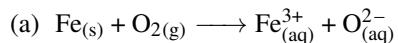
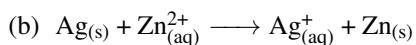
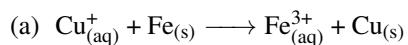
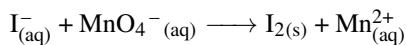
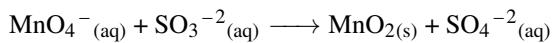
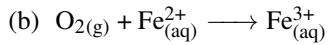
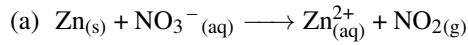
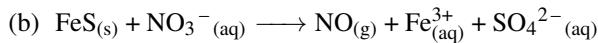
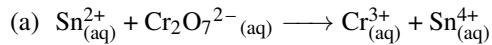
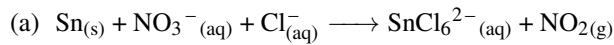
5.34 Obtain the net ionic equation for the following reaction:



5.35 Obtain the net ionic equation for the following reaction: $2\text{Na}_3\text{PO}_{4\text{(aq)}} + 3\text{CaCl}_{2\text{(aq)}} \longrightarrow 6\text{NaCl}_{(\text{aq})} + \text{Ca}_3(\text{PO}_4)_{2\text{(s)}} \downarrow$

5.36 Obtain the net ionic equation for the following reaction:



**REDOX****5.37** Balance the following redox reactions:**5.38** Balance the following redox reactions:**5.39** Balance the following redox reactions in acidic medium:**5.40** Balance the following redox reactions in acidic medium:**5.41** Balance the following redox reactions in acidic medium:**5.42** Balance the following redox reactions in basic medium:**5.43** Balance the following redox reaction in basic medium:



Ch. 6. Reactions in gase phase

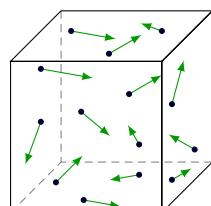
THE air we all breathe contains numerous gases, such as oxygen, nitrogen, or carbon dioxide. Some of these gases are indeed essential for life. As an example, plants take up carbon dioxide to give off oxygen, and water is produced by the reaction of oxygen and hydrogen gas. Other gases are dangerous for life. An example is carbon monoxide, which results from gas stoves, heating systems, and fire. This is a colorless, odorless, and tasteless gas that can bind to the blood displacing oxygen. As a consequence, carbon monoxide can build up in closed environments causing death. This chapter deals with the properties of gases. You will learn how to calculate the volume or pressure of a gas, characterizing its state. You will also learn how to work with mixtures of gases and for example predict the pressure of oxygen in an atmosphere containing numerous gases.

6.1 Gases and its properties

Gases contain atomic or molecular particles. They have very different properties than liquids or solids. The particles of a gas are spread and far away from each other. Liquids, on the other hand, are made of loose particles that interact through weak forces. Solids, on the other hand, are packed materials, and their particles, atoms, or molecules, are closer together. This section covers the different properties of gases.

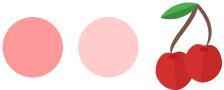
Gases in the periodic table Some of the elements in the periodic table are molecular gases, resulting from the combination of two atoms of the same element. For example, molecular oxygen (O_2) is a gas. Similarly, molecular nitrogen (N_2), molecular hydrogen (H_2), molecular chlorine (Cl_2), or molecular fluorine (F_2) are all diatomic gases—they contain two atoms of the same element. Other gases result from the combination of two different non-metals. Examples are carbon monoxide (CO) or dioxide (CO_2), and nitrogen monoxide (NO) or dioxide (NO_2). The noble gases (Ne , He , Ar) also exist in the gas state.

Characteristics of gases Gases have different properties compared to solids or liquids:



▲Microscopic picture of a gas

- Gases assume the volume and shape of their container. As they expand, they have no shape different than their container's shape.
- Gases are compressible: they can be compressed, reducing their volume. Differently, liquids and solids are incompressible.
- The density of gases is small, compared to the one for solids and liquids.



Volume, V The volume of a gas (V) is the amount of space it occupies, and gases fully occupy the volume of their container. Liters (L) and milliliters (mL) are units of volume. A liter is a cubic unit and one litter equals a cubic decimeter (dm^3).

Temperature, T The temperature (T) of a gas is related to the speed (the average velocity) of its particles. The higher the temperature the higher the particles' speed. Although there are different units of temperature such as Kelvin (K) or celsius (C°), in this chapter many formulas require the use of Kelvin temperature (T_K), that related to celsius (T_C) by the formula

$$T_K = T_C + 273$$

▼ Chlorine reactive is a gas



▼ Hydrogen is a flammable gas used to power some cars



Figure 6.1 All gas elements; some monoatomic others diatomic molecules. For example, oxygen is found as O_2 , and hydrogen as H_2 . Differently, Neon is found as a monoatomic gas.

Amount of gas, n The amount of a gas (n) refers to the number of gas particles. The larger the amount of gas, the larger the number of gas particles. The amount of gas is measured in moles or grams. Figure 6.1 displays a list of all gas elements.

Pressure, P In general, pressure is defined as force divided by surface. In the international system, the unit of force is the Newton (N) and the unit of area (A) is the m^2 . One newton is $1\text{kg} \cdot \text{m/s}^2$.

$$P = \frac{F}{A}$$

The particles of a gas are constantly moving. On their movement, they frequently hit the walls of their container, like raindrops hitting the ceiling when it rains. When they hit the walls they exert pressure, and pressure is defined as the force acting on a certain area. The larger pressure the stronger the collisions with the walls and the higher the frequency of collision—the stronger the force applied to the walls. Imagine you are driving a motorcycle. While you drive you can feel the collision of the air's particles with your face. The faster you go the higher pressure. The value of air pressure is measured with a barometer and depends on your location on the earth—in particular your altitude—as well as the weather. If you are at sea level the atmospheric pressure is one unit of pressure (one atm), due to the air that you have on top of you. If you climb a mountain, the pressure decreases, as there is less air on top of you. The higher you are from the sea level, the lower the air pressure. The weather also affects pressure, and

on hot days the pressure of air is higher, whereas on cold days pressure is lower. Units of pressure are bars, atmospheres (atm), torr, pascals (Pa), or millimeters of mercury (mmHg). To convert pressure units, you can use the following conversion factors:

1 atm
1.01325 bar

$\frac{1 \text{ atm}}{760 \text{ mmHg}}$

$$\frac{1 \text{ torr}}{1 \text{ mmHg}}$$

1 atm
101325 Pa

one millimeter of mercury (mmHg) is the same as 1 torr. As a note, the name torr acknowledges the person who invented the barometer: Torricelli, an Italian physicist. The US equivalent to 1 atm is 14.7 psi. For example, the pressure inside the tires of a car ranges from 30 to 35 psi.

Sample Problem 59

An oxygen sample has a pressure of 2 atm. Convert this value to: (a) mmHg and (b) Pascals.

SOLUTION

(a) we start by placing the given data (2 atm) and using the conversion factor between atm and mmHg, with the atm unit on the bottom, so that the units cancel

$$2 \text{ atm} \times \frac{760 \text{ mmHg}}{1 \text{ atm}} = 1520 \text{ mmHg}$$

(b) we proceed as in (a) but using the conversion between atm and Pa:

$$2 \text{ atm} \times \frac{101325 \text{ Pa}}{1 \text{ atm}} = 2.02 \times 10^5 \text{ Pa}$$

◆ STUDY CHECK

An oxygen sample has a pressure of 730 mmHg. Convert this value to atmospheres.

▼A barometer used to measure the atmospheric pressure



▼A manometer used to measure gas pressures

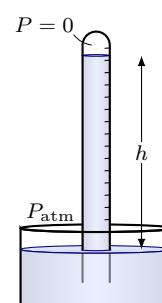


▼A pressure gauge



Figure 6.2 Pressure measuring devices

Measuring pressure Two different devices are used to measure pressure, barometers, and manometers. Barometers are used to measure specifically the atmospheric pressure and historically, they consist of a glass tube filled with mercury (Hg), inverted on a plate containing more mercury. At sea level, the height of the mercury columns should be close to 760mmHg. Manometers, on the other hand, are used to measure the pressure of any gas. Manometers consist of a u-shaped tube filled with mercury. There are two types of manometers: open-tube and closed-tube manometers. The pressure exerted by a gas changes the level of mercury on both sides of the tube and the height difference measured as the right minus the left side ($\Delta h = h_{right} - h_{left}$) is related to the gas pressure. For closed-tube manometers—normally used to measure pressure below the atmospheric pressure—when the gas pressure increases the left column of the barometer is reduced and the right column increases. The difference between both



▲A barometer, in a closed glass tube the pressure of the atmosphere is the same as a downward pressure of a mercury column.



columns is related to the gas pressure through:

$$P_{closed} = hgd \quad P_{open} = hgd + P_{atm} \quad (6.1)$$

where:

P is the pressure of the gas in Pa

Δh is the height difference in m, measured as $h_{right} - h_{left}$

d is the density of mercury 13593 kg/m^3

g is gravity, 9.8 m/s^2

P_{atm} is the atmospheric pressure close to 101325 Pa

For the open-tube manometer, normally used to measure pressure above the atmospheric pressure, we need to take into account the atmospheric pressure to the gas pressure. For this type of manometer, if the left column is below the right column ($\Delta h = h_{right} - h_{left} < 0$), this means that the pressure in the gas is below the atmospheric pressure.

The atmosphere is made of oxygen (21%), nitrogen (78%) as well as other minor gases (1%). These particles exhibit a pressure on us called atmospheric pressure. This pressure changes with altitude and with the weather. On a hot day, the column of air on top of us has more particles, and pressure increases. On a rainy day, the atmospheric pressure exerts less pressure. Above the sea level or at high altitudes the atmospheric pressure is less than 760 mmHg. For example, at mount Everest, the atmospheric pressure can be as low as 253 mmHg.

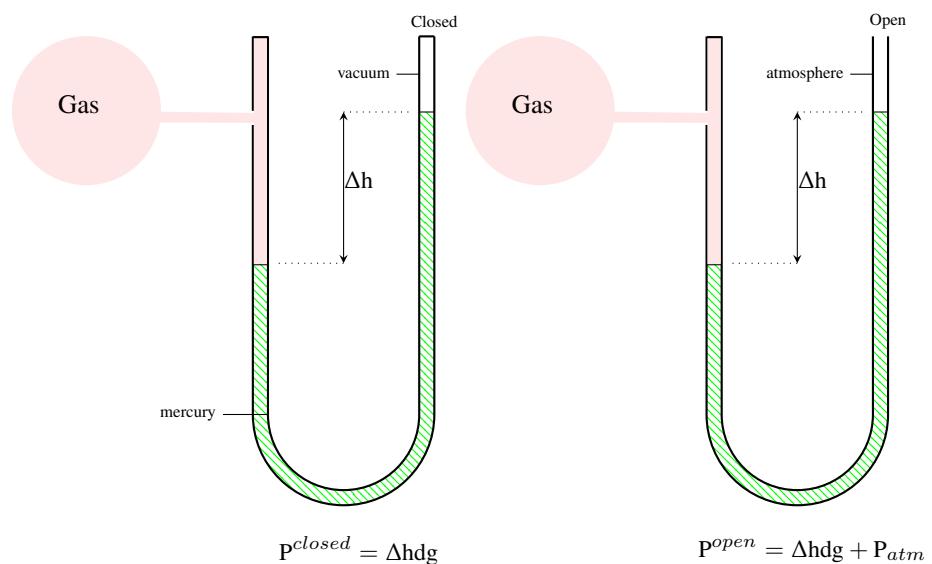
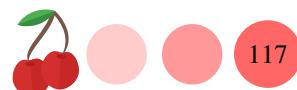


Figure 6.3 Two types of manometers: open-tube and closed-tube manometer

6.2 Ideal gas law

Ideal gases are gases made of particles without a size (very tiny) that do not interact with each other. The temperature, pressure, volume, and number of moles of a gas are not independent. They are related through the ideal gas law. In this section, we will introduce this law in two different forms: in terms of volume and terms of density.



Ideal gas law in terms of moles The ideal gas law says:

$$PV = nRT \quad \text{Ideal Gas Law}$$

where:

P is the pressure of the gas in atm

V is the volume of the gas in L

n is the number of moles of the gas

T is the temperature of the gas in K

R is the constant of the gas $0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}}$

Imagine for example that you inflate a balloon with your mouth, introducing air particles into the balloon. While the number of particles inside the balloon grows, its volume will grow too. More particles will collide with the walls of the balloon and hence, the pressure inside the balloon will also increase.

Sample Problem 60

Helium gas is used to inflate blimps, scientific balloons and party balloons. What is the volume in liters of a 0.2 moles Helium balloon at 300K and 2 atm.

SOLUTION

Analyze the Problem	Given	Asking
	$T = 300K$ $P = 2\text{atm}$ $n = 0.2\text{mol}$ $R = 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}}$	V

Using now the ideal gases formula: $PV = nRT$, we have

$$2\text{atm} \cdot V = 0.2\text{mol} \cdot 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}} \cdot 300\text{K}$$

All units but L cancel out. Solving for V we have 2.46 L.

❖ STUDY CHECK

What is the pressure in atmospheres of a 1 L balloon containing 3 moles of Helium at 40°C.

Ideal gas law in terms of density The ideal gas law in terms of density is:

$$P \cdot MW = DRT \quad \text{Ideal Gas Law in terms of D}$$

where:

P is the pressure of the gas in atm

MW is the molecular weight (or atomic weight, AW) of the gas in g/mol

D is the density in $\text{g} \cdot \text{L}^{-1}$

T is the temperature of the gas in K



R is the constant of the gas $0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}}$

We use this formula when we are questioned about the molar mass or density of the gas.

Sample Problem 61

What is the density of a Helium balloon at 400K and 3 atm.

SOLUTION

Besides the data in the problem, as the gas is He we already know its atomic mass from the periodic table:

Analyze the Problem	Given	Asking
	$T = 400\text{K}$ $P = 3\text{atm}$ $AW = 4\text{g} \cdot \text{mol}^{-1}$ $R = 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}}$	D

Using now the ideal gases formula in terms of density: $P \cdot MW = DRT$, we have

$$3\text{atm} \cdot 4 \frac{\text{g}}{\text{mol}} = D \cdot 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}} \cdot 400\text{K}$$

Solving for D we have $0.36 \text{ g} \cdot \text{L}^{-1}$.

❖ STUDY CHECK

What is the molecular mass of a $4 \text{ g} \cdot \text{L}^{-1}$ density gas at 30°C and 5 atm.

STP conditions STP conditions refer to standard temperature (273K) and pressure (1 atm) conditions. Working at STP conditions means the pressure will be fixed at 1 atm and temperature at 273K.

1 atm and 273K **STP Conditions**

Sample Problem 62

Calculate the volume in liters of 5 moles of nitrogen at STP conditions.

SOLUTION

From the problem we have the following data:

Analyze the Problem	Given	Asking
	$n = 5\text{moles}$ $P = 1\text{atm}$ $T = 273\text{K}$	V

We need to apply the ideal gas formula with the set of given variables:

$$1\text{atm} \cdot V = 5\text{mol} \cdot 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}} \cdot 273\text{K}$$

and solving for V we have a final volume of 112L.

❖ STUDY CHECK

Calculate the grams in 4L of N_2 at STP conditions.

6.3 Change of gas properties

The previous section addressed the properties of an ideal gas. However, as all properties of a gas are related, if we modify one the others will change too. This section covers situations in which one of the gas properties changes (e.g. V changes) and you need to predict the change of another gas property (e.g. P). For example, imagine you compress a balloon with your hand. The temperature and number of moles of the gas inside the balloon are constant, as the balloon is closed and in contact with the atmosphere. Differently, the pressure and volume will change. In particular, the volume will decrease and the pressure will increase. This means that the gas particles will hit the balloon harder and with more frequency.

Solving problems with an initial and final state To solve problems in which two of the gas variables are kept fixed and the other two are fixed, one needs to apply the ideal gas law at the initial and final state to then divide both formulas. Imagine a situation in which you have a 1L hot air balloon with 1 mole of gas and you add gas to a total of 5 moles. You want to calculate the final volume after you inflate the volume, knowing the temperature and pressure are kept constant. The initial state corresponds to 1L and 1 mole of gas and the final estate corresponds to an unknown volume and 5 moles. Using the ideal gas formula twice you have:

$$\left. \begin{array}{l} PV_1 = n_1 RT \\ PV_2 = n_2 RT \end{array} \right\} \frac{PV_1}{PV_2} = \frac{n_1 RT}{n_2 RT} \quad (6.2)$$

as some of the variables cancel out:

$$\frac{P'V_1}{P'V_2} = \frac{n_1 RT}{n_2 RT} \quad (6.3)$$

and you end up with Avogadro's law. If you plug the numbers into the formula:

$$\frac{1L}{V_2} = \frac{1 \text{ mol}}{5 \text{ mol}} \quad (6.4)$$

and you get a final volume of 5L.

Sample Problem 63

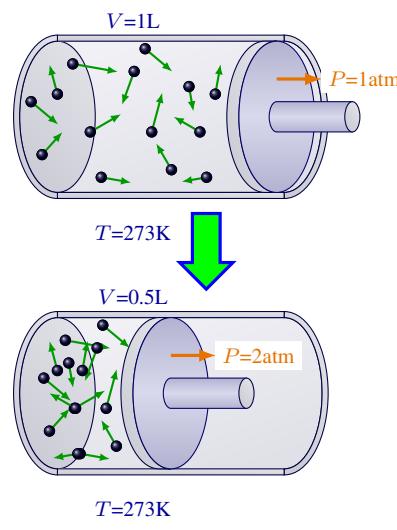
A 3L gas sample has a pressure of 5 atm. If the pressure increases to 10 atm at fixed temperature and number of moles, calculate the final volume of the gas.

SOLUTION

From the problem we have the following data:

	Given	Asking
Analyze the Problem	$V_1 = 3L$ $P_1 = 5 \text{ atm}$ $P_2 = 10 \text{ atm}$	V_2

We need to apply the ideal gas formula to the initial state and final state and divide both formulas. The number of moles and the temperature are constant



▲ Boyle's Law



and will cancel out from both equations:

$$\left. \begin{array}{l} P_1 V_1 = nRT \\ P_2 V_2 = nRT \end{array} \right\} \frac{P_1 V_1}{P_2 V_2} = \frac{nRT}{nRT} \quad (6.5)$$

Plugging the values:

$$\frac{P_1 V_1}{P_2 V_2} = \frac{nRT}{nRT} \quad (6.6)$$

and solving:

$$\frac{3 \cdot 5}{10 \cdot V_2} = 1 \quad (6.7)$$

the final volume will be 1.5 L.

◆ STUDY CHECK

A 4 atm gas sample has a temperature of 300K. If we decrease its temperature to 200K at fixed volume and number of moles, calculate the final pressure of the gas.

Pressure-Volume change If temperature and the number of moles of gas are kept constant the product of pressure and volume will remain constant too. This is the case of the balloon-pressing example. We call this Boyle's Law:

$$\frac{P}{V} = c \quad \text{or} \quad P_1 \cdot V_1 = P_2 \cdot V_2 \quad \text{Boyle's law}$$

where:

P_1, V_1 are the initial pressure and volume

P_2, V_2 are the final pressure and volume

c is a constant

Pressure-Temperature change Imagine you cool down a balloon at a fixed volume. What would happen to the balloon's pressure? Based on Gay-Lussac's law, its pressure will decrease:

$$\frac{V}{T} = c \quad \text{or} \quad \frac{P_1}{T_1} = \frac{P_2}{T_2} \quad \text{Gay-Lussac's law}$$

where:

P_1, T_1 are the initial pressure and temperature

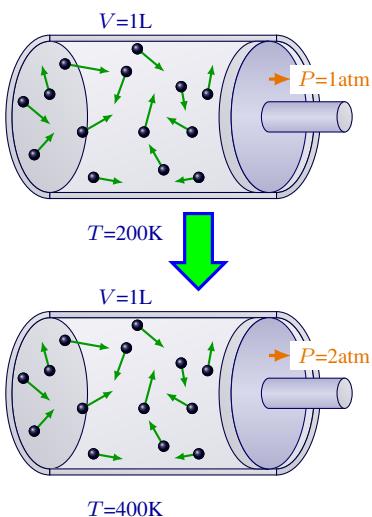
P_2, T_2 are the final pressure and temperature

c is a constant

Volume-Temperature change Imagine you cool down a balloon at a fixed pressure (under the atmosphere). What would happen to the balloon's volume? Based on Charle's law, its volume will decrease:

$$\frac{V}{T} = c \quad \text{or} \quad \frac{V_1}{T_1} = \frac{V_2}{T_2} \quad \text{Charle's law}$$

where:



▲ Gay-Lussac's Law

V_1, T_1 are the initial volume and temperature

V_2, T_2 are the final volume and temperature

c is a constant

Volume-Moles change Imagine a hot air balloon. Air comes in and out of the balloon as the balloon is not closed. Hence the pressure inside the balloon is just the atmospheric pressure. Also as the balloon is in contact with the air, its temperature will be constant, resulting from the thermal equilibrium between the inside of the balloon and the atmosphere. If you inflate the balloon with hot air, the volume of the balloon and the number of moles are related by Avogadro's law:

$$\frac{V}{n} = c \quad \text{or} \quad \frac{V_1}{n_1} = \frac{V_2}{n_2}$$

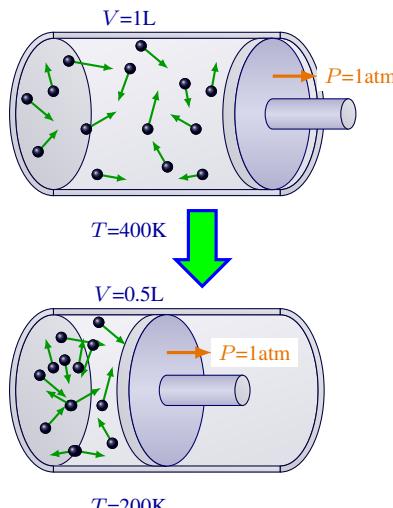
Avogadro's law

where:

V_1, n_1 are the initial volume and number of moles

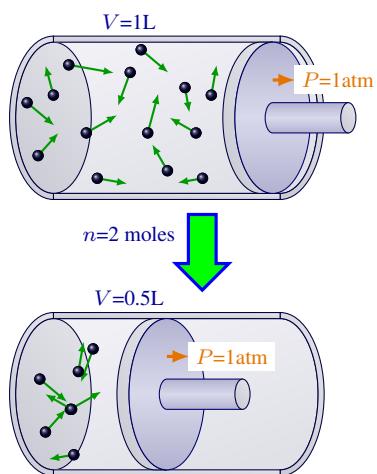
V_2, n_2 are the final volume and number of moles

c is a constant



▲ Charle's Law

Relating the different variables of a gas The question is now if we increase the pressure at a fixed number of moles and pressure, how do we know if the volume will increase or perhaps decrease? Similarly, if for example, the number of gas moles increases at fixed pressure and volume, will the temperature of the gas increase or perhaps decrease? We can answer these questions by employing the ideal gas law. If the variables that we need to relate are on the same side of the equation (e.g. P and V) then if one of the variables increases the other will decrease. Differently, If the gas variables to relate are located on opposite sides of the gas law (e.g. P and T) then both will change in the same direction. For example, let us consider the changes of P and V (at fixed n and T). As they are on the same side of the ideal gas law ($PV = nRT$) if P increases V will decrease. Differently, for the change of P and T (at fixed V and n), as both variables are on opposite sides of the ideal gas law ($PV = nRT$), if P increases, T will increase as well.



▲ Avogadro's Law

6.4 Mixtures of gases and gas stoichiometry

The air is a mixture of different gases. It contains oxygen (O_2) and nitrogen (N_2) as well as other gases such as carbon dioxide, argon, or water vapor. Only 21% of the air is made of oxygen and 78.2% of nitrogen. The other gases represent 0.8% of the air. The atmospheric pressure is 1 atm and results from the pressure of all the components of the air. Each gas exerts a partial pressure and all combined exert the total atmospheric pressure. In this section, you will learn how to work with mixtures of gases. This section also covers the use of the molar volume to relate moles and volume at standard conditions.

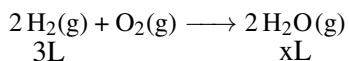
Molar volume If we work at STP conditions the volume of one mole of gas equals 22.4L, and we refer to this relationship as the molar volume.

$$\frac{1\text{mol}}{22.4\text{ L at STP}} \quad \text{Molar Volume}$$

This relationship allows us to carry out stoichiometric calculations in a chemical reaction involving gases.



Stoichiometry and gases If you encounter chemical reactions with gases, the molar volume relation allows you to carry out stoichiometric calculations. Why is this important? Imagine you have this reaction:



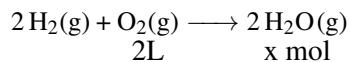
Gases are measured using their pressure and are more convenient to speak about liters of hydrogen than moles of hydrogen or grams of hydrogen, as hydrogen is a gas. This way, if we start by mixing 3L of H₂ we would like to know how much water is being produced. To calculate this, we will use the stoichiometric coefficients. In previous chapters, we saw that these numbers represent moles and the units of these numbers are mol. If the reaction deals with gases you want to interpret the stoichiometric coefficients in terms of liters. This way:

$$x = 3 \cancel{\text{L of H}_2} \times \frac{2 \text{ L of H}_2\text{O}}{2 \cancel{\text{L of H}_2}} = 3 \text{ L of H}_2\text{O}.$$

Overall, if we mix three liters of hydrogen we obtain 3L of water. In case we know the liters of any of the reactants and we need to calculate the moles of product, then we have to add an extra step to transform liters into moles.

Sample Problem 64

Hydrogen gas reacts with oxygen gas to produce water vapor according to the following equation:



Calculate the number of moles of water produced from 2L of oxygen at STP conditions.

SOLUTION

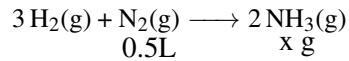
We will solve the problem in a single line, first relating the liters of oxygen and liters of water produced and finally converting liters of water into moles of water using the molar volume. Remember when there are gases in the reaction, the stoichiometric coefficients can be interpreted in terms of liters:

$$x = 2 \cancel{\text{L of O}_2} \times \frac{2 \cancel{\text{L of H}_2\text{O}}}{2 \cancel{\text{L of O}_2}} \times \frac{1 \text{ mol of H}_2\text{O}}{22.4 \cancel{\text{L of H}_2\text{O}}} = 0.178 \text{ mol of H}_2\text{O}.$$

We have that two liters of oxygen produce four liters of water. At the same time, 22.4L of water—or any other gas—is 1 moles of that gas. So four L of water are 0.17moles of water.

◆ STUDY CHECK

Hydrogen gas reacts with nitrogen (MW=28 g/mol) gas to produce ammonia (MW=17 g/mol) at STP conditions according to the following equation:



Calculate the number of grams of ammonia produced from 0.5L of nitrogen.

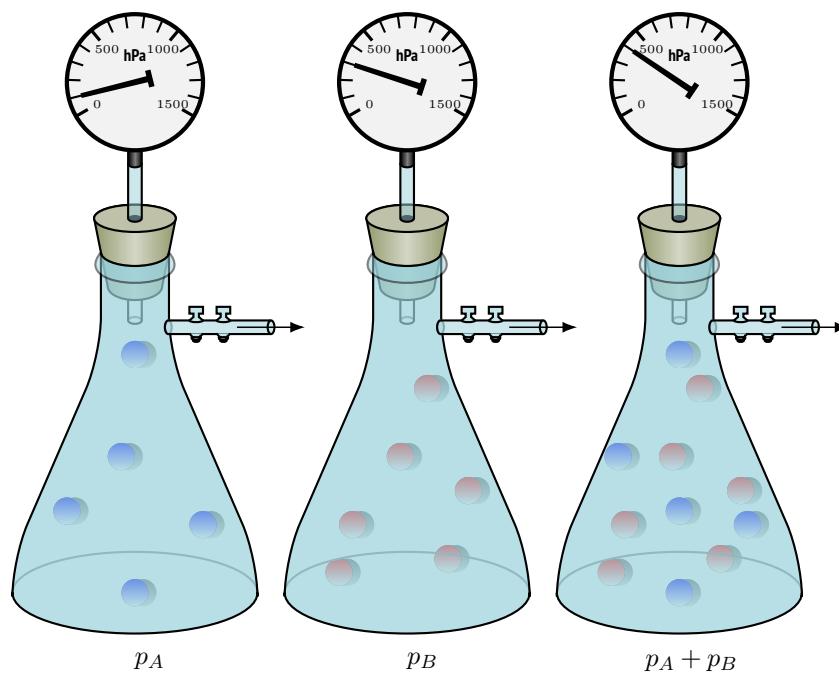


Figure 6.4 A visual representation of Dalton's law of partial pressure: after adding two different gases with different partial pressures, the final pressure is the result of adding both partial pressures.

Partial and total pressure Imagine you have a container with 1 atm of Ar and another container of the same volume containing 1 atm of Ne. If you combine the containers into a single container (and the temperature does not change), hence the pressure in the container will result from both gases and will be 2 atm. Inside the mixed container, 2 atm will be the total pressure (P_{Total}), whereas the partial pressure of each gas (p_1 and p_2) will be 1 atm. Dalton's Law says that the total pressure results from adding the partial pressure of each gas. For a gas mixture with n components:

$$P_{Total} = p_1 + p_2 + \dots + p_n \quad \text{Dalton's Law}$$

Sample Problem 65

Medical Air is an odorless gas made mostly of nitrogen and oxygen, administered by ventilator in hospital settings with an operating gauge pressure of 3 atm. If the oxygen pressure inside a container is 2.37 atm, calculate the partial pressure of nitrogen in the mixture.

SOLUTION

The problem gives the total pressure of the mixture and the partial pressure of one of the components. By using Dalton's law, we know that if the total pressure is 3 atm and the partial pressure of oxygen is 2.37, hence the partial pressure of the other component has to be 0.63 atm.

❖ STUDY CHECK

Entonox is a medicinal mixture of dinitrogen oxide (N_2O) and oxygen (O_2). The pressure N_2O in an entonox container is 2 atm and the oxygen pressure is 1520 mmHg as well. Calculate the total pressure in atm in an Entonox container.



Partial pressure of a gas in a mixture For a mixture with different gases, the partial pressure of a given gas (A) will depend on the number of moles of that particular gas and the overall volume of the mixture

$$p_A = \frac{n_A RT}{V}$$

Mole fraction The mole fraction (X_A) of a gas (A) in a mixture of gas is just the number of moles of this gas over the total number of moles in the mixture. The larger the mole fraction of a gas in a mixture the more molecules of that specific gas are there in the mixture. One can express the mole fraction in terms of partial pressures also, as the pressure of a given gas over the total pressure. For a mixture with n components:

$$X_A = \frac{n_A}{n_A + n_B + \dots + n_n} \quad \text{or} \quad \frac{p_A}{p_A + p_B + \dots + p_n}$$

For a mixture of gases, the partial pressure of a gas (p_A) is related to the mole fraction of that gas (X_A) and the total pressure of the mixture of gases (P_{Total}):

$$p_A = X_A \cdot P_{Total}$$

Sample Problem 66

A mixture of gases with a total pressure of 2 atm contains 3 moles of Ar, 3 moles of He and 1 moles of Ne. Calculate the partial pressure of each component on the mixture.

SOLUTION

We calculate first the mole fraction for each component of the mixture. As the total number of moles is 7 moles and there are 3 moles of Ar, its mole fraction is 0.43. Similarly, the mole fraction for He is 0.43 and for Ne is 0.14. To calculate the partial pressure of each gas you just need to multiply its mole fraction by the total pressure (2 atm). Hence: $p_{Ar}=0.86\text{atm}$, $p_{He}=0.86\text{atm}$ and $p_{Ne}=0.28\text{atm}$

◆ STUDY CHECK

A mixture of gases with a total pressure of 5 atm contains 1 mol of Ar and 1 mol of He. Calculate the partial pressure of each component on the mixture.

6.5 Collecting gas over water

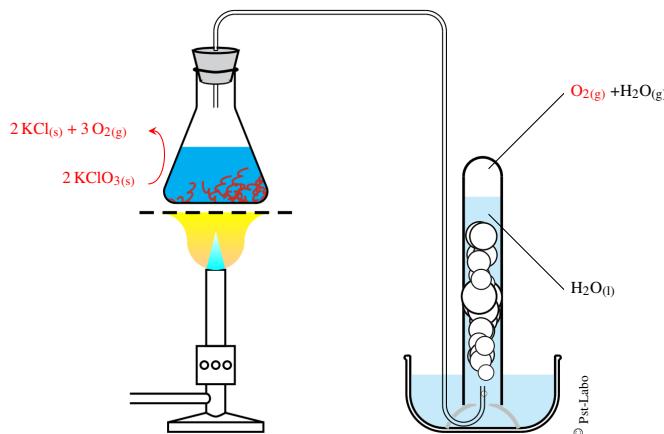


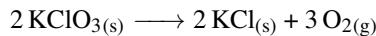
Figure 6.5 Apparatus for measuring the amount of gas produced by a reaction over water.

Table 6.1 Vapor pressure, partial water pressure as a function of temperature

T°C	P(atm)								
5	0.0086	25	0.0313	45	0.0946	65	0.2469	85	0.5706
10	0.0121	30	0.0419	50	0.1218	70	0.3077	90	0.6920
15	0.0168	35	0.0555	55	0.1555	75	0.3806	95	0.8342
20	0.0231	40	0.0728	60	0.1967	80	0.4675	100	1.0000

Collecting gas over water: use of partial pressures

Numerous reactions produce gases. As an example, potassium chlorate decomposes to produce oxygen gas:



The volume of gas produced by a chemical reaction is collected often over water. Gas bubbles go through water being collected in an apparatus similar to the one represented in Figure 6.5.

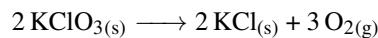
As the gas is collected over water, with the gas produced by the reaction, we will also find water molecules that will exhibit a certain partial pressure. In other words, we will collect a mixture of two gases, the gas produced by the reaction and water. The partial pressure of the gas produced will be:

$$P_{\text{gas}} = P_{\text{total}} - P_{\text{H}_2\text{O}}$$

The partial pressure of water, also called the vapor pressure of water, depends on temperature and its values can be found in Table 6.1. For example, at 25°C, the vapor pressure of water in the atmosphere is 0.0313 atm and at 100°C is equal to 1 atm. When liquids boil, their vapor pressure is equal to the atmospheric pressure, which is the reason behind the vapor pressure of water being 1 atm at 100°C, the boiling point of water.

Sample Problem 67

Oxygen is collected over water in the decomposition of potassium chlorate:





Given that 20mL of gas are collected at 30°C at a pressure of 0.9atm, and that the vapor pressure of water at that temperature is 0.0419 atm, calculate the number of moles of oxygen collected.

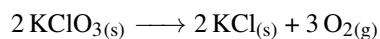
SOLUTION

In order to calculate the number of moles of oxygen collected we need the partial pressure of oxygen, the temperature and the volume. We have that as the total pressure is 0.9atm and the partial pressure of water is 0.0419 atm, then the partial pressure of oxygen should be $0.9 - 0.0419$ atm, that is 0.481 atm. As we have the temperature (303K) and the volume (0.02L), we can calculate the number of moles of oxygen:

$$n_{\text{O}_2} = \frac{P_{\text{O}_2}V}{RT} = \frac{0.481 \cdot 0.02}{0.082 \cdot 303} = 3.8 \times 10^{-4} \text{ moles of O}_2$$

◆ STUDY CHECK

Oxygen is collected over water in the decomposition of potassium chlorate:



Given that 10mL of gas are collected at 35°C at a pressure of 0.5atm, and that the vapor pressure of water at that temperature is 0.0555 atm, calculate the number of moles of KClO_3 decomposed.

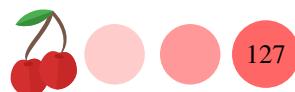
6.6 Kinetic molecular theory of gases

At this point, we know enough about the properties of gases to be able to condense all these pieces of information into a quantitative model that could generate numerical predictions. The kinetic model of gases can predict among other properties the particle average velocity—this is technically called root mean square velocity, v_{RMS} .

Kinetic theory of gases The kinetic theory of gases is a model that explains the properties of gases. This theory envisions a gas in the form of a set of moving particles. Some of the ideas behind this model are:

- The particles of a gas are in constant motion and move very fast.
- On its movement, gas particles collide with each other changing paths and colliding with the walls of their container exerting pressure.
- Gas particles are far apart from each other, barely interacting.
- The average kinetic energy of the particles of gas (this is the energy of the particles due to movement) is proportional to the temperature of the gas.

Using the kinetic theory we can rationalize the different properties of a gas. As the particles of a gas are in constant motion and apart from each other they fill and occupy the same volume of their container. The temperature of a gas is related to its kinetic energy, that is, the average speed of the gas particles. Also, as the gas particles collide with the container's wall, they exert pressure. The kinetic theory of gases explains for example how room fresheners work. As you spray the room, the molecules of the perfume in a gas state move fast and occupy the room. The kinetic molecular theory of the gases gives a molecular-based description of the temperature of a gas—among



other properties. The ideal gas law is experimental; this means is a law that comes from measuring and carrying experiments. However, this law does not provide any reasons behind the behavior of gases, ideal or real. The kinetic molecular theory provides a molecular description of temperature. In particular one of the outcomes of this theory is that the average velocity of a gas particle depends on the square root of the temperature of the gas. More precisely, the way this theory describes velocity is in the form of a *root mean square velocity* v_{RMS} , that is, as an average of the velocity of each particle. The formula that connects the root mean square velocity with temperature is:

$$v_{RMS} = \sqrt{\frac{3000RT}{MW}}$$

root mean square velocity formula

where:

MW is the molecular weight of the gas in g/mol

T is the temperature of the gas in K

R is the constant of the gas in energy units $8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

v_{RMS} is the root mean square velocity in m/s

It is important to notice that the root mean square velocity depends on temperature—the more temperature the more velocity—and is inversely proportional to the molecular weight of the gas—the heavier the mass the lower velocity.

Sample Problem 68

Order the following molecules in increasing order of root mean square velocity:

Ne, CO₂ and H₂O.

SOLUTION

Root mean square velocity is inversely proportional to the molecular weight of the gas; hence, the larger the mass the lower velocity. If we compare the molecular weight of the gases: Ne(MW=20g/mol), CO₂(MW=44g/mol) and H₂O(MW=18g/mol). The root mean square velocity of water is the largest and the root mean square velocity of carbon dioxide is the smallest.

◆ STUDY CHECK

Calculate the root mean square velocity of the molecules of water at 25°C.

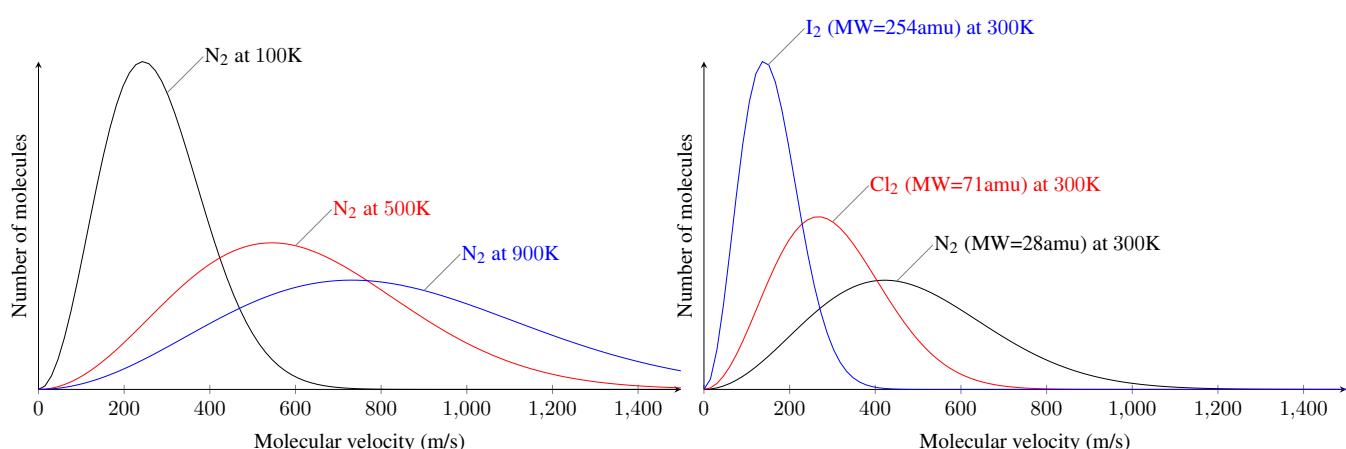


Figure 6.6 Effect of temperature and mass on the distribution of molecular speeds



Distribution of velocities The root means square velocity v_{RMS} is just an average of the square velocities of the gas particles. Still, some particles will have faster velocity than v_{RMS} , and others will have slower velocity. The molecular velocities of the particles of gas follow a distribution that is mass and temperature dependent. As shown in Figure 6.6, the higher temperature the larger the root square velocity, with a wider distribution of velocities. At the same time, the larger the molar mass of the gas, the smaller the root square velocity with a thinner distribution of velocities.

6.7 Real gases

Until now we have discussed ideal gases. These simplistic representations of gases represent very dilute gases in which the gas particles are apart. The particles of an ideal gas are also considered to be very minute without a volume. At the same time, the collisions between the particles and the walls of the container are elastic—this means the molecules do not lose any energy. As you can imagine, no gas is an ideal gas, as this is just an ideal model. This section will cover the properties of real gases, in which the gas particles interact among themselves and the collisions are inelastic and energy is lost.

Van der Waals equation for real gases When we take into account the fact that the particles of a gas interact with each other the formula of the ideal gases does not work anymore. Instead, we can use the Van der Waals equation for real gases that functions in a very similar way.

$$P = \frac{nRT}{V - nb} - \frac{n^2a}{V^2}$$

Van der Waals equation

where:

P is the pressure of the gas in atm

V is the volume of the gas in L

n is the number of moles of the gas

T is the temperature of the gas in K

R is the constant of the gas $0.082 \frac{\text{atm}\cdot\text{L}}{\text{mol}\cdot\text{K}}$

a and b are the Van der Waals constants in units of $\text{atm}\cdot\text{L}^2\cdot\text{mol}^{-2}$ and $\text{L}\cdot\text{mol}$

Table 6.2 Van der Waals constants for several gases

gas	a ($\text{atm}\cdot\text{L}^2/\text{mol}^2$)	b (L/mol)	gas	a ($\text{atm}\cdot\text{L}^2/\text{mol}^2$)	b (L/mol)
NH_3	4.225	0.0371	Ar	1.355	0.03201
C_6H_6	18.24	0.1154	CO	3.640	0.04267
CH_4	2.283	0.0427	CH_3OH	9.649	0.06702
CS_2	11.77	0.0768	Cl_2	6.579	0.05622
Ne	0.2135	0.01709	NO	1.358	0.02789
N_2	1.370	0.0387	NO_2	5.354	0.04424

The meaning of the Van der Waals constants There are two Van der Waals constants: a and b (see Table 6.2). The Van der Waals constant a represents



the degree of interaction between the molecules of a gas. The larger these values the more interactions exist between the gas particles. For example, for He we have $a = 0.0341 \text{ atm} \cdot \text{L}^2 / \text{mol}^2$, whereas for H₂O we have $a = 5.46 \text{ atm} \cdot \text{L}^2 / \text{mol}^2$. Comparing the values of a for both gases, we can conclude that the interaction between the particles of He is very weak and in contrast, the interactions between the particles of H₂O are stronger. The Van der Waals constant b is related to the molecular size, however, the relationship is not as straightforward as in the case of the a constant.

Sample Problem 69

Calculate the pressure of 0.2 moles of water vapor at 500K occupying a volume of 0.1L, using: (a) the ideal gas formula and (b) the Van der Waals formula $a = 5.46 \text{ atm} \cdot \text{L}^2 / \text{mol}^2$ and $b = 0.0305 \text{ L/mol}$.

SOLUTION

We will use the ideal gas formula first, given the number of moles ($n=0.2 \text{ mol}$), temperature ($T=500\text{K}$), pressure ($p=6 \text{ atm}$) and the volume ($V=0.1\text{L}$).

$$P = \frac{nRT}{V} = \frac{0.2 \times 0.083 \times 500}{0.1} = 82 \text{ atm}$$

Now, using the Van der Waals formula:

$$P = \frac{nRT}{V - nb} - \frac{n^2a}{V^2} = \frac{0.2 \times 0.083 \times 500}{0.1 - 0.2 \times 0.0305} - \frac{0.2^2 \times 5.46}{0.1^2} = 65 \text{ atm}$$

Both values are very different and this is consistent with the fact that water vapor does not behave as an ideal gas.

◆ STUDY CHECK

Calculate the pressure of 0.9 moles of ammonia gas at 900K occupying a volume of 0.1L, using: (a) the ideal gas formula and (b) the Van der Waals formula $a = 4.17 \text{ atm} \cdot \text{L}^2 / \text{mol}^2$ and $b = 0.0371 \text{ L/mol}$.

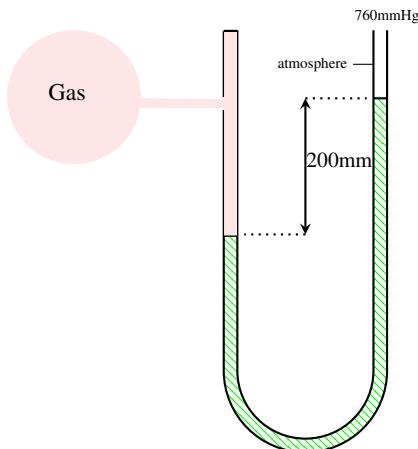
CHAPTER 6

GASES AND ITS PROPERTIES

6.1 Convert the following properties: (a) A pressure value of 2 atm into mmHg (b) A pressure value of 3000 Pa into atm (c) A temperature value of 25°C into K

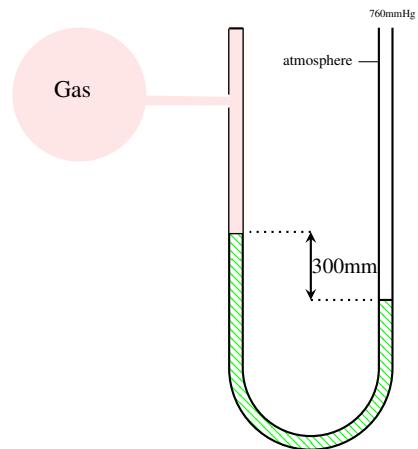
6.2 Convert the following properties: (a) A pressure value of 900 mmHg into torr (b) A temperature value of 400K into °C

6.3 An open-tube manometer is used to measure the pressure of a given gas. When there is no gas in the container, the mercury levels are equal in both sides of the u-tube.



(a) Would the gas pressure be lower or higher than the atmospheric pressure? (b) Calculate the gas pressure in MPa. (c) Calculate the gas pressure in Torr.

6.4 An open-tube manometer is used to measure the pressure of a given gas. When there is no gas in the container, the mercury levels are equal in both sides of the u-tube.



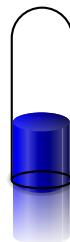
(a) Would the gas pressure be lower or higher than the atmospheric pressure? (b) Calculate the gas pressure in MPa. (c) Calculate the gas pressure in Torr.

6.5 A barometer is a device used to measure the atmospheric pressure. It is made of a glass tube filled with a liquid, inverted on a dish of the same liquid. When inverting the tube, liquid will remain on the tube. The filled height of the column is proportional to the pressure. The liquid used is normally mercury with density 13593 kg/m³.



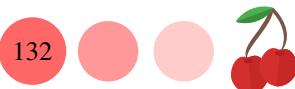
(a) Calculate the atmospheric pressure in atm if you use a barometer containing a liquid of density 1000 kg/m³ and the liquid height is 9cm. (b) What are the drawbacks of building a barometer with a lighter liquid than mercury?

6.6 A barometer is a device used to measure the atmospheric pressure. It is made of a glass tube filled with a liquid, inverted on a dish of the same liquid. When inverting the tube, liquid will remain on the tube. The filled height of the column is proportional to the pressure. The liquid used is normally mercury with density 13593 kg/m³.



(a) Given that the height of the column is 750mm, calculate the atmospheric pressure in MPa. (b) What are the benefits of building a barometer with a lighter liquid than mercury?

IDEAL GAS LAW



6.7 A gas contained in a 3L tank has a pressure of 5 atm at a temperature of 400 K. Calculate the number of moles in the tank.

6.8 Dinitrogen oxide, used in dentistry, is an anesthetic also called laughing gas. What is the pressure in atm of 0.35 moles of N_2O at 22°C in a 5L container?

6.9 A 4 moles sample of gas at 400K has a pressure of 10 atm. Calculate the volume of the sample.

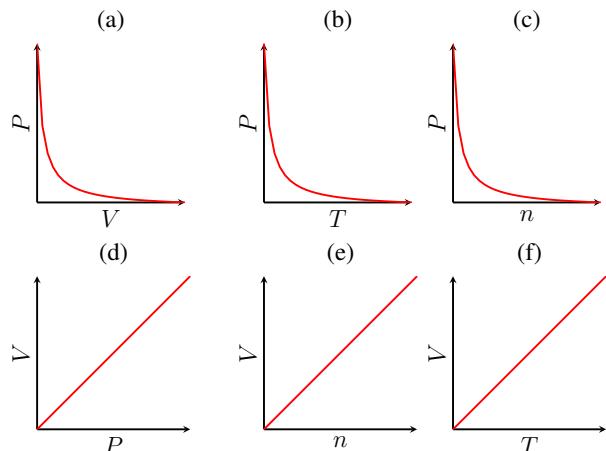
6.10 A 3 grams sample of Ar at 40°C is placed in a 3L container. Calculate the pressure inside the container.

6.11 Eighteen grams of a gas in a 11L container at 400K exert a pressure of 3 atm. Calculate the molar mass of the gas.

6.12 What is the molar mass of a gas if a 3.16 g sample at 0.75 atm and 45°C occupies a volume of 2L.

6.13 Answer the following questions: (a) Calculate the volume of a 4 moles of Ar at STP conditions. (b) Calculate the volume of a 4 moles of Ne at STP conditions. (c) Calculate the moles of gas in 3L of Ar at STP conditions. (d) Calculate the volume of 64 g of O₂ gas at STP (273K, 1atm)

6.14 Indicate what plot (or plots) below best represent the following gas laws: (a) Boyle's law (b) Charle's law (c) Avogadro's law



CHANGE OF GAS PROPERTIES

6.15 A sample of a gas at 400K and 12 atm is cooled in the same container to 200K. Calculate the new pressure.

6.16 In a storage area where the temperature has reached 300K, the pressure of oxygen gas in a 15 L steel cylinder is 1 atm. Calculate the volume if the pressure is reduced to 0.5 atm.

6.17 A closed H₂ sample has a volume of 5 L and a pressure of 1 atm. What is the new pressure if the volume is decreased to 2L with no change in temperature and the amount of gas.

6.18 A sample of Ne in a closed, expandable container, has a volume of 3L at 40°C . Calculate the new volume if the container is cooled to 25°C .

6.19 Complete the following statement: if the pressure of a gas increases, at fixed temperature and moles, its volume....

6.20 Complete the following statement: if the temperature of a gas increases, at fixed volume and moles, its pressure....

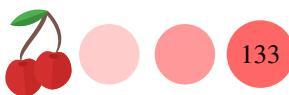
MIXTURE OF GASES AND GAS STOICHIOMETRY

6.21 A tank contains Ne gas at 700 mmHg, Ar at 2 atm, and Kr at 700 torr. What is the total pressure of the mixture in atm?

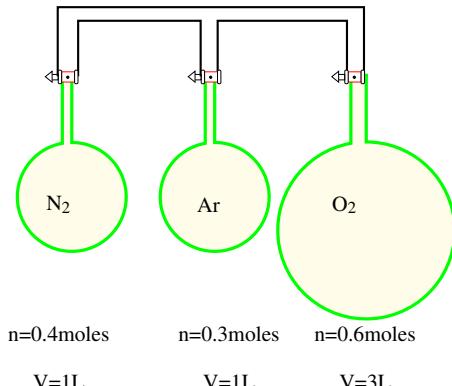
6.22 An anesthetic consist of a mixture of cyclopropane gas and oxygen gas. If the mixture has a total pressure of 2 atm and the partial pressure of cyclopropane is 0.5atm, what is the partial pressure of O₂?

6.23 The atmospheric pressure on a hot day is 780 mmHg. Given that the air is made of 78% of nitrogen and 22% of oxygen, calculate the partial pressure of each gas in the air.

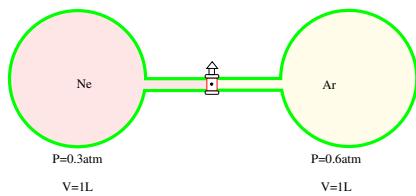
6.24 The atmospheric pressure on a hot day is 790 mmHg. Given that the air is made of 78% of nitrogen and 22% of oxygen, calculate the partial pressure of each gas in the air.



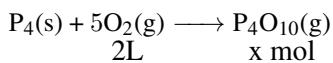
6.25 Consider the set up below with three different gases in three different closed containers at 300K. Assuming that the connecting tubes have zero volume, once the flasks are connected, calculate: (a) The partial pressure of each gas in the mixture (b) The total gas pressure



6.26 Consider the set up presented below, where the connecting tubes have negligible volume. Calculate the partial pressure of each gas after the connection between the flasks is open.

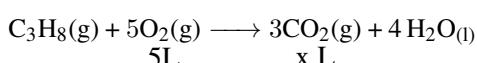


6.27 Phosphorus reacts with oxygen gas to produce tetraphosphorus decaoxide according to the following equation:

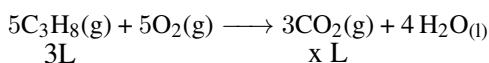


Calculate the number of moles of phosphorus that react with 2L of oxygen at STP conditions.

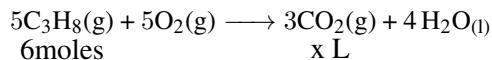
6.28 For the following reaction, calculate the unknown x at STP conditions:



6.29 For the following reaction, calculate the unknown x at STP conditions:



6.30 For the following reaction, calculate the unknown x at STP conditions:



REAL GASES AND THE KINETIC MOLECULAR THEORY OF GASES

6.31 What is the pressure in atm of 1 mol of He at 600K in a 1L container: (a) Using the ideal gas law (b) Using the real gas law given $a = 0.0342 \text{ atm} \cdot \text{L}^2/\text{mol}^2$ and $b = 0.0237 \text{ L/mol}$

6.32 Calculate the pressure p in atm exerted by 2 moles of methane (CH_4) in a 0.5L container at 300K. (a) Using the ideal gas law p^{ideal} (b) Using the real gas law p^{real} , given $a = 2.283 \text{ atm} \cdot \text{L}^2/\text{mol}^2$ and $b = 0.04278 \text{ L/mol}$ (c) Calculate the percent error in the ideal gas law using $|p^{ideal} - p^{real}|/p^{real} \times 100$.

6.33 Use the Van der walls constant a to compare which of the gases exhibit stronger intermolecular interactions between its particles for the following pair of gases: (a) Ar or Ne (b) CO or NO

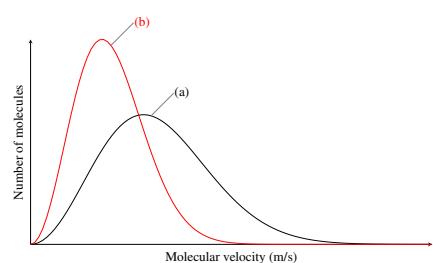
6.34 Without consulting the values of the Van der walls constant b indicate which of the gases of the following pair would exhibit a larger b value: (a) C_2H_6 or CH_4 (b) H_2 or CH_4

6.35 What is the rms speed of O_2 at STP?

6.36 Order the following molecules in increasing order of root-mean square velocity: Ne, CO_2 , H_2O , CH_4 .

6.37 Which of the following statements is assumed by the kinetic molecular theory of gases: (a) gas particles interact with each other (b) gas particles have large sizes (c) particles move slowly (d) gas particles move randomly

6.38 For the velocity distribution curved below: (a) The plots represent the distribution of velocity of two gases Ne or Ar at STP conditions in a fixed volume. What line represents each gas? (b) The plots represent the distribution of velocity of a gas at two different temperatures 300K and 500K at fixed pressure and volume conditions. What line represents each each temperature?



Ch. 7. Thermochemistry



ENERGY involves many aspects of our everyday life. Chemical reactions happening in our bodies consume or release energy as we walk, study, and even breathe. We also use energy at home to warm food or turn on the lights, drive our cars, and go to work. The energy needed for our body to function comes from food. If we do not eat for a while, we run low on energy. Similarly, the burning of fossil fuels such as oil, propane, or gasoline provides enough energy to maintain our homes. On the other hand, how do we measure the energy released or consumed in a chemical process? This chapter will answer this and other questions as it covers different aspects of the interplay between chemistry and energy. You will learn about temperature, heat, and how an energy exchange implies changes in temperature.

7.1 Energy

When you are running, walking, dancing, or thinking, you are using energy to do work. Energy is defined as the ability to do work. Suppose you are climbing a steep hill. Perhaps you become too tired to go on; you do not have sufficient energy to do any more work. Now suppose you sit down and have lunch. In a while, you will have obtained energy from the food, and you will be able to do more work and complete the climb. Similarly, chemical energy is the energy stored in the structure of chemicals and it depends on the arrangement of molecules and the nature of these molecules.

Potential & Kinetic Energy: *heat* Energy can be classified as potential energy or kinetic energy. Kinetic energy is the energy of motion and any fast-moving object has kinetic energy. Think about a bullet coming out of a gun; as the bullet moves very fast it contains kinetic energy that can be released when it collides with a target. Potential energy is energy stored in objects located at a certain height. A boulder resting on top of a mountain has potential energy because of its location. If the boulder rolls down the mountain, the potential energy becomes kinetic energy. Water stored in a reservoir has potential energy. When the water goes over the dam, the potential energy is converted to kinetic energy. The potential energy resulting from the interaction of charged particles is called electrostatic energy. Heat refers to thermal energy, which is associated with the random motion of particles in a substance and therefore is related to kinetic energy. A frozen pizza feels cold because the particles in the pizza are moving slowly. As the pizza receives heat, the motion of the particles increase. Eventually, the particles have enough energy to make the pizza hot and ready to be eaten. When a substance receives heat it gets warmer and it raises its temperature, whereas if it loses heat it gets cooler and its temperature decreases.



▼Flowers convert sunlight into chemical energy



© www.wallpaperflare.com

▼a bullet has kinetic energy



© www.wallpaperflare.com

▼water on a dam has potential energy



© wikipedia

▼thermal energy refers to heat



© wikipedia

Mechanical energy: work The sum of potential and kinetic energy is called mechanical energy. Mechanical energy refers to the ability to do work. Examples of work are a car engine moving or a balloon expanding its volume.

The law of conservation energy In this chapter, we will analyze energy changes associated with chemical reactions. To do this, we need to define the system and its surroundings. The system will be the chemical reaction often happening in a beaker, whereas the surroundings would be the area surrounding the beaker. The system plus its surroundings are called the universe. The beaker may lose energy, and in that case, energy will flow from the system to the surroundings. Similarly, the system may gain energy, flowing from the surroundings to the beaker. In a closed system, the energy is conserved and when one type of energy disappears, a different type of energy will appear. As an example, if you drop an object from the top of a building, originally the object had potential energy that converts into kinetic energy as the object gains speed. This is called the law of conservation of energy.

Energy units Two different units of energy are often employed: calories (cal) and joules (J). Joule is the SI unit of energy equal to $\text{kg} \cdot \text{m}^2/\text{s}^2$. One can transform calories into joules and joules into calories using the following conversion factor:

$$1\text{cal} = 4.184\text{J} \quad \text{or} \quad \frac{1\text{cal}}{4.184\text{J}} \quad (7.1)$$

As a note, often you will read on food labels the caloric content of certain foods. In these labels, they use the unit Calorie, with capitalized C, which is not the same as a calorie. One Calorie represents a kilocalorie and contains 1000 calories.

Sample Problem 70

Convert the following energy values:

$$(a) 50000\text{ cal} \text{ to Kcal} \qquad (b) 48001\text{ J} \text{ to cal}$$

SOLUTION

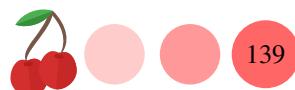
We will use the conversion factor for kilo and the relationship between calorie and joule:

$$(a) 50000\text{cal} \times \frac{1\text{kcal}}{1000\text{cal}} = 50\text{kcal}; (b) 48000\text{J} \times \frac{1\text{cal}}{4.184\text{J}} = 11472\text{cal}.$$

◆ STUDY CHECK

Convert the following energy units: (a) 200 cal to Kcal (b) 7000 J to cal

Thermodynamics Thermochemistry is a subject of a broader field called thermodynamics, which studies the interconversion of energy (heat and other types) and mass. Thermodynamics study systems, like chemical reactions. The term system, refers to the part of the universe being study. Systems can be classified as: open, closed and isolated systems. An open system can exchange mass and energy with its surroundings, whereas a closed system can only exchange mass and not energy. Isolated systems cannot exchange neither mass nor energy with its surroundings. The state of a system is characterized by the values of its volume, pressure, temperature, energy and composition, so that if a system receives heat it will change its state. Energy, volume, pressure and temperature are called state functions—or state properties—, as these properties are determined by the state of the system, independently of the path used to reach that state. In another words, these properties are path-independent. For example, in a building, the floor location of a person would be a state function, as it would not matter the path the



person took to reach that state. In contrast the amount of effort to make it to a specific floor will not be a state function, as it changes depending on the path used.

7.2 Temperature

Temperature indicates how hot or cold a substance is compared to another substance. Heat always flows from a substance with a higher temperature to a substance with a lower temperature until the temperatures of both are the same. When you drink hot coffee or touch a hot pan, heat flows to your mouth or hand, which is at a lower temperature. When you touch an ice cube, it feels cold because heat flows from your hand to the colder ice cube. Three units of temperature often employed are celsius ($^{\circ}\text{C}$, T_C), Fahrenheit ($^{\circ}\text{F}$, T_F) or Kelvin (K, T_K). If you need to convert temperature units from Fahrenheit to celsius or from celsius to Fahrenheit you need to use the formulas below:

$$T_F = 1.8T_C + 32 \quad T_F = 1.8T_K - 459.4 \quad T_K = T_C + 273 \quad (7.2)$$

Sample Problem 71

Convert $25\ ^{\circ}\text{C}$ to $^{\circ}\text{F}$.

SOLUTION

- Step one:** list of the given variables.

Analyze the Problem	Given	Asking
	$T_c = 25\ ^{\circ}\text{C}$	T_F

- Step two:** use the formula $T_F = 1.8T_C + 32$ to convert from $^{\circ}\text{C}$ to $^{\circ}\text{F}$.

- Step three:** solve for $T_F = 1.8 \times 25 + 32 = 77\ ^{\circ}\text{F}$.

◆ STUDY CHECK

Convert $200\ ^{\circ}\text{C}$ to K.

7.3 From energy to temperature

Heat transforms in a temperature change. Some substances like metals can increase their temperature very quickly with a small amount of heat received, whereas others need a larger amount of heat to rise their temperature. Think about why you use oil to deep fry food. Why not use water? First of all, oil can raise its temperature very quickly and on top of that it does not boil easily.

Heat capacity The heat capacity c of a material is defined as:

$$c = \frac{\text{heat adsorbed}}{\text{temperature increase}} \quad (7.3)$$



This is a characteristic property of each material that indicates the energy required to rise its temperature and can be expressed in cal/°C or J/°C units. As this property depends on the amount of matter, oftentimes the heat capacity is expressed per mass as the specific heat capacity also known as *specific heat* (c_e) or mole unit as the *molar heat capacity* c_m . For example, the specific heat of water is 1cal/g°C that is the same as 4.184J/g°C. That means that we need to give 1 calorie to warm up one gram of water 1°C. Similarly, the specific heat of aluminum, a metal, is 0.2cal/g°C or 0.89J/g°C; that means the energy needed to raise the temperature of an aluminum gram is 0.2 calories of 0.89 J. Mind the difference between these two values: we need to give 1 cal to increase the temperature of a gram of water in 1°C, whereas we need to give 0.2 cal to increase the temperature of a gram of aluminum in 1°C. Why are these two numbers so different? The answer is that water and aluminum are different materials. Normally metals warp up very easily, that is, they need less heat to increase their temperature, whereas liquids need more heat to increase their temperature. That is why pans and cooking pots tend to be metallic. Table 7.1 lists specific heats of common substances. Mind the specific heat if water is a well known value that you need to be familiar with:

$$c_e^{\text{H}_2\text{O}} = 4.184\text{J/g}^\circ\text{C} \quad \text{or} \quad c_e^{\text{H}_2\text{O}} = 1\text{cal/g}^\circ\text{C} \quad (7.4)$$

Table 7.1 Values of specific heat for different materials

Material	Specific heat (J/g°C)	Material	Specific heat (J/g°C)
H ₂ O _(l)	4.184	Fe _(s)	0.444
ethyl alcohol _(l)	2.460	Au _(s)	0.129
vegetable oil _(l)	1.790	Cu _(s)	0.385
NH ₃ _(l)	4.700	H ₂ O _(s)	2.010
Dry Air _(g)	1.0035	CO ₂ _(g)	0.839

Heat When a material receives heat, that heat normally becomes temperature as the temperature of the material increases. For example, if you warm milk in a microwave, the milk's temperature increases from room temperature (25°C) to a higher temperature. How to estimate the temperature increase given the heat received? Or how to estimate the heat needed to increase the temperature of an object? We can use the following formula:

$$Q = m \cdot c_e \cdot (T_f - T_i) \quad (7.5)$$

where:

Q is the amount of heat received, either in cal or J.

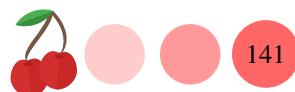
m is the mass of material in grams

c_e is the specific heat of the material (in cal/g°C or J/g°C)

$T_f - T_i = \Delta T$, is the temperature change from the initial to the final temperature

A system can receive or give away heat and this is indicated by the sign of Q . The sign convention for heat is:

$Q > 0$ the system receives heat and $Q < 0$ the system gives away heat



Sample Problem 72

How many calories are absorbed by a 45.2g piece of aluminum ($c_e = 0.214 \frac{\text{cal}}{\text{g}^\circ\text{C}}$) if its temperature rises from 25°C to 50°C .

SOLUTION

- Step one:** list of the given variables.

Analyze the Problem	Given	Asking
	$c_e = 0.214 \frac{\text{cal}}{\text{g}^\circ\text{C}}$	Q
	$m = 45.2\text{g}$	
	$T_{\text{initial}} = 25^\circ\text{C}$	
	$T_{\text{final}} = 50^\circ\text{C}$	

- Step two:** use the formula $Q = m \cdot c_e \cdot (T_{\text{final}} - T_{\text{initial}})$ to transform the temperature increase into heat absorbed. Mind this formula depends on the mass involved and the specific heat of the material, in this case, aluminum.

- Step three:** solve $Q = 45.2 \cdot 0.214 \cdot (50 - 25) = 241.82\text{cal}$.

◆ STUDY CHECK

How many calories are absorbed by 100g of Gold ($c_e = 0.0308 \frac{\text{cal}}{\text{g}^\circ\text{C}}$) if its temperature rises from 25°C to 100°C .

In the previous example you needed to convert temperature into heat. In the next example, the heat is given and you need to calculate the final temperature of an object after it receives a certain amount of heat.

Sample Problem 73

A 50g piece of aluminum ($c_e = 0.214 \frac{\text{cal}}{\text{g}^\circ\text{C}}$) initially at 25°C absorbs 100cal. Calculate the final temperature of the aluminum piece.

SOLUTION

- Step one:** list of the given variables.

Analyze the Problem	Given	Asking
	$c_e = 0.214 \frac{\text{cal}}{\text{g}^\circ\text{C}}$	T_{final}
	$m = 50\text{g}$	
	$T_{\text{initial}} = 25^\circ\text{C}$	
	$Q = 100\text{cal}$	

- Step two:** use the formula $Q = m \cdot c_e \cdot (T_{\text{final}} - T_{\text{initial}})$ that converts temperature increase to heat absorbed.



3 **Step three:** solve $100 = 50 \cdot 0.214 \cdot (T_{final} - 25)$ for T_{final} :

$$\begin{aligned} 100 &= 50 \cdot 0.214 \cdot (T_{final} - 25) && \text{divide by 50 in both sides} \\ \frac{100}{50} &= 0.214 \cdot (T_{final} - 25) && \text{divide by 0.214 in both sides} \\ \frac{100}{50 \cdot 0.214} &= (T_{final} - 25) \\ 9.34 &= (T_{final} - 25) && \text{add 25 in both sides} \\ 9.34 + 25 &= T_{final} \\ 34.34 &= T_{final} \end{aligned}$$

The final temperature of the aluminum piece is 34.34°C .

❖ STUDY CHECK

A 200g piece of iron ($c_e = 0.1 \frac{\text{cal}}{\text{g} \cdot ^{\circ}\text{C}}$) initially at 15°C absorbs 1000cal. Calculate the final temperature of the metal piece in $^{\circ}\text{C}$.

7.4 The first law of thermodynamics

Materials can absorb heat and receive work. On one hand, think about a pizza in your oven, or a cup of milk in the microwave. These substances receive heat from the oven or in form of microwaves and they become hot. Heat transforms in an increase in temperature. On the other hand, if you hammer a wall, the wall receives work from you, and this work is translated to energy as the wall may break. Work and heat are both combined in a property called internal energy, E .

Work Think about what happens to a car's engine. In an engine, chemical energy is converted into movement and with this movement, a car can carry work. Work (W) is force (F) applied over a distance (Δh):

$$W = F \cdot \Delta h = (P \cdot A) \cdot \Delta h$$

For the case of a gas confined in a cylindrical container, force is related to pressure times area (A). Therefore, if the pressure is constant as $A \cdot \Delta h$ equals to volume (V), we have that

$$W = -P \cdot \Delta V \quad (7.6)$$

where:

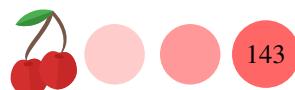
W represents work

P is the pressure

ΔV is the change of volume calculated as $V_{final} - V_{initial}$

The minus sign is just a convention, as in chemistry the work done by the surroundings to a system is considered positive, as the system gains work (energy). Therefore, when ΔV is negative because the system receives work, the value of W has to be positive. In another word, the sign convention for work is:

$W > 0$ the system receives work and $W < 0$ the system gives away work



As a final note, the type of work that involves a change in volume at constant pressure is normally called PV work.

Sample Problem 74

Calculate the work (in L · atm) involved in the expansion of a gas from 10L to 20L at constant external pressure of 2atm. Convert the value in joules using $101.3\text{J}=1\text{L} \cdot \text{atm}$.

SOLUTION

We will use Equation 7.6 that related work with pressure and volume change:

$$W = -P \cdot \Delta V = -2\text{atm} \cdot (20 - 10)\text{L} = -20\text{L} \cdot \text{atm}$$

If we convert this value into J:

$$-20\text{L} \cdot \text{atm} \times \frac{101.3\text{J}}{1\text{L} \cdot \text{atm}} = -2026\text{J}$$

As the value is negative, it means that the system gives away work.

◆ STUDY CHECK

Calculate the work involved in the compression of a gas from 10L to 5L at constant external pressure of 5atm (a) in L · atm units, and (b) in joules, using $101.3\text{J}=1\text{L} \cdot \text{atm}$.

First law of thermodynamics: the internal energy The combination of work (W) and heat (Q) is called internal energy (ΔE):

$$\Delta E = Q + W \quad (7.7)$$

The first law of thermodynamics—the law of conservation of energy—states that the energy of the universe is constant.

Sample Problem 75

When a hot balloon inflates and deflates in order to change its height. It receives 10^3J of heat and its volume increases from $3.0 \times 10^5\text{L}$ to $3.5 \times 10^5\text{L}$ at fixed external pressure of 1atm. Calculate the internal energy of the hot balloon, using $1\text{J}=101.3\text{L} \cdot \text{atm}$.

SOLUTION

We will use Equation 7.6 that related work with pressure and volume change. As the resulting unit of work will be L · atm, we will directly convert the value into J:

$$W = -P \cdot \Delta V = -1\text{atm} \cdot (3.5 \times 10^5 - 3.0 \times 10^5)\text{L} \times \frac{1\text{J}}{101.3\text{L} \cdot \text{atm}} = -493.6\text{J}$$

Now we will add the value of heat (10^3J) to the value of work to calculate the internal energy:

$$\Delta E = Q + W = 10^3 + (-493.6) = 1493.6\text{J}$$

Overall, the hot balloon receives more heat than the work it gives away and hence the resulting internal energy is positive—the system gains energy.

◆ STUDY CHECK

When a hot balloon deflates, it receives 10^7J of work from the external atmo-



sphere and its temperature change from 90°C to 25°C. Given that the air initially contained in the balloon has a mass of $3 \times 10^5 \text{ g}$ and a specific heat of $1 \text{ J/g}^\circ\text{C}$. Calculate the internal energy of the hot balloon.

7.5 Calorimetry

A calorimeter is a tool used to measure the exchange of heat happening in chemical reactions and calorimetry is the science that measures heat exchange by using calorimeters. There are two types of calorimeters, very fancy and expensive ones called constant-volume calorimeters, and more affordable ones, in the form of a coffee cup, called constant-pressure calorimeters (see Figure 7.1).

The calorimeter A calorimeter is a device used to measure the energy exchanged in a chemical reaction—we call this molar heat of reaction, ΔQ_r . In essence, a calorimeter is a closed system that does not let the heat come through its walls. By measuring the temperature change inside the calorimeter we can compute the energy exchange in a chemical reaction happening inside the calorimeter. If the temperature inside a calorimeter increases, this means that the reaction releases energy. On the contrary, if the temperature inside a calorimeter decreases, this means the reaction consumes energy. There are two different types of calorimeters: constant pressure and constant-volume calorimeters. As a note, ΔQ_r is called the molar heat of the reaction as it represents energy per mole, with units of kJ/mol.

Constant-pressure calorimeter A constant-pressure calorimeter is the simplest of all calorimeters and is called constant pressure as the pressure inside the calorimeter is constant and equal to the atmospheric pressure. A constant-pressure calorimeter is just a double coffee cup covered with a lid. Inside this cup, a chemical reaction occurs in a liquid phase. If the reaction produces any gases as the cup is just covered with a lid, the pressure will always be equal to the atmospheric pressure as the gas can escape through the lid. The formula used in calorimetry with a constant-pressure calorimeter has only two terms. Let us use a reaction that produced heat as an example. Inside a constant-pressure calorimeter, you introduced two reagents, and a reaction happens, producing heat. The heat exchanged from the reaction (first term) changes the temperature of the liquid inside the calorimeter (second term). At the same time, we assume that the walls of the calorimeter do not absorb heat. The formula used in calorimetry with a constant-pressure calorimeter is the following:

$$0 = n \cdot \Delta Q_r + \Delta Q_{water} \quad \text{constant pressure}$$

where:

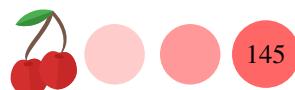
$n \cdot \Delta Q_r$ is the heat exchanged due to a chemical reaction

ΔQ_{water} is the heat received or released by water

The water contribution is given by the heat formula given above. After we plug the formula of the heat into the formula above we arrive at the constant-pressure calorimetry formula:

$$0 = n \cdot \Delta Q_r + V \cdot d \cdot c_e^{\text{sol}} \cdot (T_f - T_i) \quad \text{constant pressure}$$

where:



ΔQ_r is the heat exchanged due to a chemical reaction in J/mol

n is the number of moles of the limiting reagent

V is the volume of water in mL contained in the calorimeter

d is the density of the solution in g/mL

c_e^{sol} is the specific heat of the solution: tend to be similar to water, $4.184\text{J/g}^\circ\text{C}$

$T_f - T_i = \Delta T$, is the temperature change from the initial to the final temperature

Sample Problem 76

We mix 5mL of NaOH 0.5M with 5mL of HCl 0.5M both at 25°C in a constant-pressure calorimeter. The final temperature inside the calorimeter is 27°C . Calculate the heat of reaction if the solution density is 1g/mL and the specific heat of the solution is $4.184\text{J}/^\circ\text{C}$.

SOLUTION

Analyze the Problem	Given	Asking
	$n = 5 \times 10^{-3}\text{L}$ $0.5\text{M} = 2.5 \times 10^{-3}\text{moles}$ $V = 10\text{mL}$ $d = 1\text{g/mL}$ $T_f = 27^\circ\text{C}$ $T_i = 25^\circ\text{C}$ $c_e^{\text{H}_2\text{O}} =$ $4.184\text{J/g}^\circ\text{C}$	ΔQ_r

We have all data needed to solve the calorimetry formula. We have the moles of the limiting reagent, the overall volume of the mixture, the density of the mixture, the temperature change and the specific heat of the solution. Plugging all values into the calorimetry formula we have:

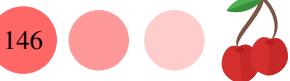
$$0 = n \cdot \Delta Q_r + V \cdot d \cdot c_e^{\text{sol}} \cdot (T_f - T_i)$$

$$0 = 2.5 \times 10^{-3}\text{mol} \cdot \Delta Q_r + 10\text{g} \cdot 4.184\text{J/g}^\circ\text{C} \cdot (27^\circ\text{C} - 25^\circ\text{C})$$

Solving for ΔQ_r we obtain -33472J/mol that is the same as -33.5KJ/mol . As the value is negative, it means that the reaction produced energy and hence is exothermic.

❖ STUDY CHECK

We mix 2.5mL of NaOH 0.5M with 2.5mL of HCl 0.5M both at 25°C in a constant-pressure calorimeter. The heat of reaction is -40KJ/mol . Calculate the final temperature inside the calorimeter, if the solution density is 1g/mL and the specific heat of the solution is $4.184\text{J/g}^\circ\text{C}$.



▼A constant-volume calorimeter



© wikipedia

▼A constant-pressure calorimeter



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Figure 7.1 Different types of calorimeters. A constant-volume calorimeter is also called a bomb calorimeter. A constant-pressure calorimeter is also called a coffee-cup calorimeter

Constant-volume calorimeter A constant-volume calorimeter—also known as a bomb calorimeter—is a more complex and costly calorimeter in which normally gas phase reactions occur. This type of calorimeter is rigid and even if gas is produced the volume of the container will not change—that is why it is called a constant-volume calorimeter. Constant-volume calorimeters are used to calculate the energy value of food—and for example, calculate the calories in a bag of chips. The formula to carry calorimetric calculations with a constant-volume calorimeter has three terms: the first term represents the energy exchanged due to the reaction, the second term represents the energy exchanged by water in the calorimeter, and the last term represents the heat exchanged by the walls of the calorimeter. The formula used in a constant-volume calorimeter is the following:

$$0 = n \cdot \Delta Q_r + \Delta Q_{water} + \Delta Q_{walls}$$

where:

$n \cdot \Delta Q_r$ is the heat exchanged due to a chemical reaction

ΔQ_{water} is the heat received or released by water

ΔQ_{walls} is the heat absorbed by the walls

$$0 = n \cdot \Delta Q_r + m \cdot c_e^{\text{H}_2\text{O}} \cdot (T_f - T_i) + c^{\text{cal}} \cdot (T_f - T_i)$$

Constant-volume

where:

ΔQ_r is the heat exchanged due to a chemical reaction in J/mol

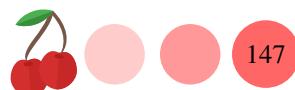
n is the number of moles that reacted inside the calorimeter

m is the mass of water contained in the calorimeter

$c_e^{\text{H}_2\text{O}}$ is the specific heat absorbed of water: $4.184 \text{ J/g}^\circ\text{C}$

c^{cal} is the heat capacity of the calorimeter also known as the calorimeter factor

$T_f - T_i = \Delta T$, is the temperature change from the initial to the final temperature



Sample Problem 77

A 3 mol-sample of a chemical is burned in a constant-volume calorimeter with 10g of water and a heat capacity of 10KJ/ $^{\circ}\text{C}$. Calculate the heat of reaction knowing that the initial temperature of the water inside the calorimeter is 25°C and the final 40°C .

SOLUTION

Analyze the Problem	Given	Asking
	$n = 3\text{mol}$ $m = 10\text{g}$ $T_f = 40^{\circ}\text{C}$ $T_i = 25^{\circ}\text{C}$ $c^{cal} = 10^4\text{J}/{}^{\circ}\text{C}$ $c_e^{\text{H}_2\text{O}} = 4.184\text{J/g}^{\circ}\text{C}$	ΔQ_r

We have all data needed to solve the calorimetry formula. We have the moles of chemical inside the calorimeter, the heat capacity of the calorimeter, the initial and final temperature of water, and the amount of water. Mind that the specific heat of water is always given and you need to remember the value. Also and more importantly mind that the units of the heat capacity of the calorimeter are KJ/ $^{\circ}\text{C}$, whereas the units of the specific heat of water are J/g $^{\circ}\text{C}$ and hence, we need to convert KJ into J; that is the reason we use 10000J/ $^{\circ}\text{C}$ as the heat capacity of the calorimeter. Plugging all values into the calorimetry formula we have:

$$0 = 3\text{mol} \cdot \Delta Q_r + 10\text{g} \cdot 4.184\text{J/g}^{\circ}\text{C} \cdot (40^{\circ}\text{C} - 25^{\circ}\text{C}) \\ + 10000\text{J}/{}^{\circ}\text{C} \cdot (40^{\circ}\text{C} - 25^{\circ}\text{C})$$

Solving for ΔQ_r we obtain -50209J/mol that is the same as -50.209KJ/mol . As the value is negative, it means that the reaction produced energy and hence is exothermic.

◆ STUDY CHECK

A 2 mol-sample of a chemical reacts in a constant-volume calorimeter with 20g of water and a heat capacity of 11KJ/ $^{\circ}\text{C}$. Calculate the heat of reaction knowing that the temperature of water inside the calorimeter rises 10°C .

7.6 Reactions and energy

Exothermic and endothermic reactions Some reactions release heat; these are called exothermic reactions. Others absorb heat and are called endothermic reactions. Think for example the combustion of the gas in a cooking stove. This reaction produces heat and hence it is exothermic. Differently, bread needs heat to rise. Hence, the chemical reaction involved in bread making should be endothermic. Similarly, if you melt an ice cube you need to give energy to the cube so that it becomes water. The



melting of ice is an endothermic reaction. Endothermic reactions have positive heat of reaction ΔH_R and are normally accompanied by an indication of heat in the reactants side of the reaction before the arrow.



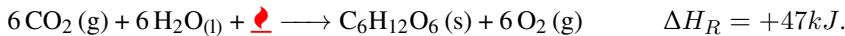
Differently, exothermic reactions normally accompanied by an expression of heat in the products side have negative ΔH_R .



Figure 7.2 represents endo and exothermic processes.

Sample Problem 7.8

Classify the following reactions as exothermic and endothermic:



SOLUTION

The first reaction is exothermic as it produces heat. Differently, the second reaction is endothermic and absorbs energy.

◆ STUDY CHECK

Classify the following reactions as exothermic and endothermic:



Heat-Mole conversions Remember that a chemical reaction can be translated into a series of conversion factors that relate the moles of reactants with the products or with other reactants. At the same time, a chemical reaction involving heat can be converted into a series of conversion factors that are related to energy and the moles of reactants and products. For the exothermic reaction:



the moles of hydrogen are related to heat:

$$\frac{2 \text{ moles of H}_2}{-572 \text{ kJ}} \text{ or } \frac{-572 \text{ kJ}}{2 \text{ moles of H}_2}$$

Similarly, we can relate energy with moles of O₂ or moles of water:

$$\frac{1 \text{ moles of O}_2}{-572 \text{ kJ}} \text{ or } \frac{-572 \text{ kJ}}{1 \text{ moles of O}_2}$$

$$\frac{2 \text{ moles of H}_2\text{O}}{-572 \text{ kJ}} \text{ or } \frac{-572 \text{ kJ}}{2 \text{ moles of H}_2\text{O}}$$

We will use these relationships to convert moles of reactants or products into heat.

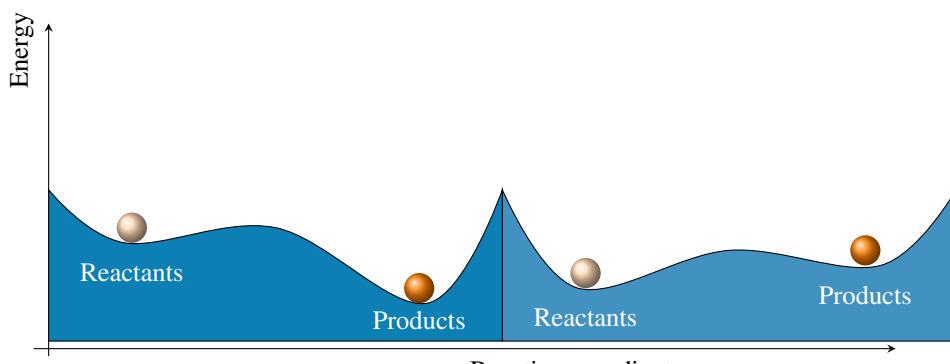
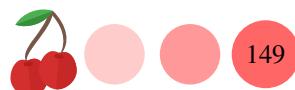


Figure 7.2 An exothermic (left) reaction and an endothermic (right) reaction.

Sample Problem 79

Hydrogen reacts with nitrogen to produce ammonia (NH_3) according to the following reaction



Calculate: (a) the enthalpy of reaction; (b) indicate whether the reaction is endo or exothermic; (c) calculate the heat exchanged when produced 5 moles of ammonia.

SOLUTION

(a) the heat of reaction is -92KJ , and (b) the reaction is exothermic as the heat appears as a product. This means the reaction produces heat. (c) We will use the conversion factor that relates ammonia with heat and will set up the moles of ammonia on the bottom of the conversion factor so that the units will cancel and energy will remain

$$5 \frac{\text{moles of NH}_3}{\text{moles of NH}_3} \times \frac{-92\text{KJ}}{2 \frac{\text{moles of NH}_3}{\text{moles of NH}_3}} = -230\text{KJ},$$

that is: 5 moles of ammonia produce -230KJ . The fact that this value is negative means that heat will be released.

◆ STUDY CHECK

Given the reaction below, calculate the number of hydrogen moles needed to generate -200KJ .



7.7 Energy value of food

Calories in food How much food do you eat? How many calories do you ingest a day? When you are watching your food intake, the Calories you are counting are kilocalories (1000cal, Kcal, or Cal). In the field of nutrition, it is common to use the Calorie, Cal (with an uppercase C) to indicate 1000 cal or 1 kcal.

$$1\text{Cal} = 1000\text{cal}$$

or

$$\frac{1\text{Cal}}{1000\text{cal}}$$

or

$$\frac{1000\text{cal}}{1\text{Cal}}$$

(7.8)

Table 7.2 Energy value of food

Food Type	Energy value ($\frac{\text{kcal}}{\text{g}}$)
Carbohydrates	4
Fat	9
Protein	4



Energy values Do you ever eat pasta? Think about how does your body feel after you eat pasta? Normally, whenever you eat pasta in a few hours you need to eat again more food. Differently, whenever you eat meat, that is enough to keep you going for a longer time. Similarly, eating a salad for lunch brings you less energy than a pizza slice. This is because each type of food—each ingredient—contains different energy. We refer to this as the energy value of food ϵ . Table 7.2 lists energy values for common ingredients. To compute the energy (E) provided by a certain mass of food (m) we need to multiply the mass times the energy value (ϵ):

$$E = m \cdot \epsilon \quad (7.9)$$

For example, the energy value of fat ϵ_{fat} is $9 \frac{kcal}{g}$, which means that if you eat three grams of fat that will bring you a given amount of energy E_{fat} :

$$E_{fat} = 3g \times 9 \frac{kcal}{g} = 18kcal$$

Normally, when you eat a food plate, you ingest energy from the different types of ingredients of that plate: fat, carbs, or protein.

Sample Problem 80

A Big Mac from McDonalds contains 28g of fat (9kcal/g), 46g of carbs (4kcal/g) and 25 g of protein (4kcal/g), where the caloric values are indicated in parenthesis. What is the total energy content of a Big Mac?

SOLUTION

- 1 **Step one:** list of the given information and the unknown.

Analyze the Problem	Given	Asking
	$m_{fat} = 28g$ $\epsilon_{fat} = 9 \frac{kcal}{g}$ $m_{carb} = 46g$ $\epsilon_{carb} = 4 \frac{kcal}{g}$ $m_{prot} = 25g$ $\epsilon_{prot} = 4 \frac{kcal}{g}$	Energy Content

- 2 **Step two:** use the formula $E_{fat} = m_{fat} \cdot \epsilon_{fat}$ to calculate the energy coming from fat. And do the same for carbs and protein.

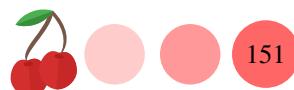
- 3 **Step three:** Compute the energy coming from each ingredient and add all the values:

$$E_{fat} = m_{fat} \cdot \epsilon_{fat} = 28g \times 9 \frac{kcal}{g} = 252kcal \quad \text{energy from fat}$$

$$E_{carb} = m_{carb} \cdot \epsilon_{carb} = 46g \times 4 \frac{kcal}{g} = 184kcal \quad \text{energy from carbs}$$

$$E_{prot} = m_{prot} \cdot \epsilon_{prot} = 25g \times 4 \frac{kcal}{g} = 100kcal \quad \text{energy from protein}$$

The total energy content of a Big Mac is: $E_{fat} + E_{carb} + E_{prot} = 532kcal$



STUDY CHECK

A pepperoni pizza slice contains 11g of fat (9kcal/g), 36g of carbs (4kcal/g) and 14 g of protein (4kcal/g), where the caloric values are indicated in parenthesis. What is the total energy content of a pizza slice?

7.8 Enthalpy

In the last section, we have seen that when a chemical reaction proceeds it exchanges energy with the surroundings. This energy can be measured in many different conditions. When it is measured at constant pressure—these are regular conditions in chemistry, think about a reaction happening at a beaker—this energy change has a different name: it is called enthalpy and is represented with the symbol ΔH_f° . In this section, we will cover the different types of enthalpies depending on the type of reaction—formation or reaction—and we will find out how to compute the enthalpy change for a reaction using tables of standard enthalpies given at the end of the chapter.

What is enthalpy? You want to think about enthalpy as heat. There are different ways to measure the heat exchanged in a system—as constant-pressure heat or constant-volume heat. Enthalpy is the constant-pressure heat. It is important in chemistry, as many chemical reactions happen at constant pressure, that is, in open containers in contact with the atmosphere. Enthalpy is indeed related to the internal energy

$$H = U + PV$$

Working under constant pressure we have

$$\Delta H = \Delta U + P\Delta V$$

as $\Delta U = Q - P\Delta V$ we have

$$\Delta H = Q_p$$

where Q_p means heat measured at constant pressure.

Table of standard enthalpies The values of enthalpies are tabulated in Table 7.4. The term standard refers to standard pressure conditions (1 atm) and is indicated by a degree sign on the top right side (ΔH°). Let us see how to use Table 7.4. If you look for the standard enthalpy of C—an element—from Table 7.4 you might find several values. The values of graphite carbon are $\Delta H_f^\circ = 0\text{KJ/mol}$. Differently, the values for diamond carbon are different than zero, being $\Delta H_f^\circ = 1.0\text{KJ/mol}$. Similarly, the value for gas carbon is not zero also, being $\Delta H_f^\circ = 716.67\text{KJ/mol}$. This is because the natural state of carbon is in the form of graphite. That is, the most common way in which we find carbon in nature is in the form of graphite and not diamond or gas. Let us find the standard enthalpy for molecular nitrogen, $\text{N}_2(\text{g})$ —another element. If you look into Table 7.4 you will find a value of $\Delta H_f^\circ = 0\text{KJ/mol}$, again because the natural state of nitrogen is in the form of gas N_2 . How much is the standard enthalpy of gas hydrogen, H_2 ? If you look in Table 7.4, the value is also $\Delta H_f^\circ = 0\text{KJ/mol}$. The rule of thumb is: elements in their natural state have zero H_f° . Below we will explain more about the meaning of the natural state. Now, look for the standard enthalpy of



carbon monoxide gas, CO(g) . The value should not be zero, as carbon dioxide is not an element and is made of two different types of atoms. Indeed, in Table 7.4 we find $\Delta H_f^\circ(\text{CO(g)}) = -110.5\text{KJ/mol}$.

Sample Problem 81

Using the enthalpy tables at the end of the chapter, locate the enthalpy values for: $\text{CaS}_{(s)}$, $\text{AlCl}_3{}_{(s)}$ and $\text{H}_2\text{O}_{(l)}$.

SOLUTION

The enthalpy of calcium sulfide in solid state ($\text{CaS}_{(s)}$) is -482.4KJ/mol . For the case of aluminum chloride in solid state too ($\text{AlCl}_3{}_{(s)}$), the enthalpy is -705.63KJ/mol . Finally, the enthalpy of liquid water is -285.8KJ/mol .

◆ STUDY CHECK

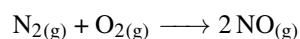
Using the enthalpy tables at the end of the chapter, locate the enthalpy values for: $\text{I}_{2(aq)}$, $\text{F}_{2(g)}$ and $\text{C}_{\text{diamond}(s)}$.

Natural state of an element The natural state of an element is the most stable state in which we find this element in nature. For example, you can find Aluminum as a solid, liquid, or gas. However, its natural state is solid, as we find Al in nature as a solid. That is the reason why $\Delta H_f^\circ(\text{Al}_{(g)}) = 314\text{KJ/mol}$, whereas $\Delta H_f^\circ(\text{Al}_{(s)}) = 0\text{KJ/mol}$. In general, metals, in their natural state is solid. For non-metallic elements, such as hydrogen, oxygen, nitrogen, fluorine, and chlorine, its natural state is in the form of a diatomic gas molecule. For example, $\Delta H_f^\circ(\text{H}_{2(g)}) = 0\text{KJ/mol}$, $\Delta H_f^\circ(\text{N}_{2(g)}) = 0\text{KJ/mol}$ or $\Delta H_f^\circ(\text{O}_{2(g)}) = 0\text{KJ/mol}$. For the case of carbon, its natural state is graphite, $\Delta H_f^\circ(\text{C}_{\text{graphite}(s)}) = 0\text{KJ/mol}$. Molecules such as H_2O or NO have standard enthalpy different than zero. Mind that molecules are not elements, and hence are made of different elements. Table 7.3 lists the standard state of common elements.

Table 7.3 Standard states for different elements. For all $\Delta H_f^\circ = 0\text{KJ/mol}$

Element	Standard state	Element	Standard state
Hydrogen	$\text{H}_{2(g)}$	Oxygen	$\text{O}_{2(g)}$
Nitrogen	$\text{N}_{2(g)}$	Chlorine	$\text{Cl}_{2(g)}$
Iron	$\text{Fe}_{(s)}$	Aluminium	$\text{Al}_{(s)}$
Carbon	$\text{C}_{\text{graphite}(s)}$	Phosphorus	$\text{P}_{4(s)}$
Fluorine	$\text{F}_{2(g)}$	Bromine	$\text{Br}_{(l)}$
Mercury	$\text{Hg}_{(l)}$	Sulfur	$\text{S}_{8(s)}$
Iodine	$\text{I}_{2(s)}$	Silicon	$\text{Si}_{(s)}$

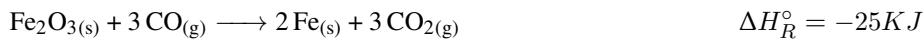
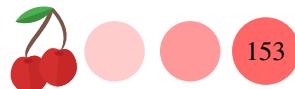
Formation reactions: standard enthalpy of formation The formation reaction starts with natural-state elements (e.g. H_2 , N_2 , etc.) to form a chemical. For example, the formation reaction of NO is given by:



On the products side, we have the chemical formed (NO) whereas on the reactant side, we have the elements that make NO in its natural state (H_2 and N_2). The enthalpy associated with this reaction is called standard enthalpy of formation $\Delta H_f^\circ(\text{NO}_{(g)})$. This value is often listed on the right of the reaction:



ΔH_R° and ΔH_f° Consider the following two reactions:



The first example represents a formation reaction and thus the enthalpy is labeled as ΔH_f° . In contrast, the second reaction is not a formation reaction. This is because the reactants are not elements in their natural state: $\text{CO}_{(\text{g})}$ and $\text{Fe}_2\text{O}_{3(\text{s})}$ have enthalpies different than zero. For this reason, the second enthalpy is labeled as ΔH_R° and is called the standard enthalpy of the reaction.

Standard enthalpy change for a reaction To calculate the standard enthalpy for a reaction you need to use the following formula:

$$\boxed{\Delta H_R^\circ = \Delta H_{\text{products}}^\circ - \Delta H_{\text{reactants}}^\circ} \quad \text{Enthalpy change}$$

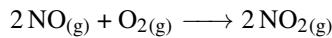
where:

ΔH_R° is the standard enthalpy change of the reaction

$\Delta H_{\text{products}}^\circ$ is the standard enthalpy of all products

$\Delta H_{\text{reactants}}^\circ$ is the standard enthalpy of all reactants

Now, imagine we need to calculate the change of standard enthalpy for the following reaction:



We need to locate three enthalpies from the table: $\Delta H_f^\circ(\text{NO}_{(\text{g})})$, $\Delta H_f^\circ(\text{O}_{2(\text{g})})$, $\Delta H_f^\circ(\text{NO}_{2(\text{g})})$. If you locate these values in the table you will see $\Delta H_f^\circ(\text{O}_{2(\text{g})}) = 0 \text{KJ/mol}$, whereas $\Delta H_f^\circ(\text{NO}_{(\text{g})}) = 90.29 \text{KJ/mol}$ and $\Delta H_f^\circ(\text{NO}_{2(\text{g})}) = 33.2 \text{KJ/mol}$. Using the formula for ΔH_R° we have:

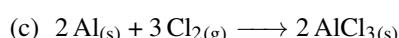
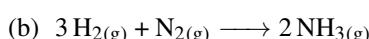
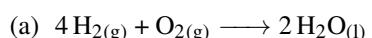
$$\Delta H_R^\circ = \Delta H_{\text{products}}^\circ - \Delta H_{\text{reactants}}^\circ =$$

$$\begin{aligned} &= [2 \cdot \Delta H_f^\circ(\text{NO}_{2(\text{g})})] - [2 \cdot \Delta H_f^\circ(\text{NO}_{(\text{g})}) + \Delta H_f^\circ(\text{O}_{2(\text{g})})] = \\ &= [2 \cdot 33.2] - [2 \cdot 90.29 + 0] = -114 \text{KJ} \end{aligned}$$

This reaction is exothermic and releases heat.

Sample Problem 82

Using the enthalpy table, calculate ΔH_R° for the following reactions:



SOLUTION

In order to answer all questions, we need a set of ΔH_f° values:

$\Delta H_f^\circ(\text{H}_{2(\text{g})})$, $\Delta H_f^\circ(\text{O}_{2(\text{g})})$, $\Delta H_f^\circ(\text{N}_{2(\text{g})})$, $\Delta H_f^\circ(\text{Al}_{(\text{s})})$ are all zero, whereas

$\Delta H_f^\circ(\text{H}_{2\text{O}(\text{l})}) = -285.8 \text{KJ/mol}$, $\Delta H_f^\circ(\text{NH}_{3(\text{g})}) = -45.0 \text{KJ/mol}$ and



$\Delta H_f^\circ(\text{AlCl}_3\text{(s)}) = -705.63 \text{ KJ/mol}$. For the first example, we have:

$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{H}_2\text{O(l)})] - [4 \cdot \Delta H_f^\circ(\text{H}_2\text{(l)}) + \Delta H_f^\circ(\text{O}_2\text{(g)})] \\ &= [2 \cdot -285.8] - [4 \cdot 0 + 0] = -572 \text{ KJ}\end{aligned}$$

For the second example:

$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{NH}_3\text{(g)})] - [2 \cdot \Delta H_f^\circ(\text{Al(s)}) + 3 \cdot \Delta H_f^\circ(\text{Cl}_2\text{(g)})] \\ &= [2 \cdot -45] - [2 \cdot 0 + 3 \cdot 0] = -90 \text{ KJ}\end{aligned}$$

Finally, for the last reaction:

$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{AlCl}_3\text{(s)})] - [3 \cdot \Delta H_f^\circ(\text{H}_2\text{(g)}) + \Delta H_f^\circ(\text{N}_2\text{(g)})] \\ &= [2 \cdot -705.63] - [3 \cdot 0 + 0] = -1411 \text{ KJ}\end{aligned}$$

◆ STUDY CHECK

Using the enthalpy table, calculate ΔH_R° for the following reaction:



7.9 Hess's Law: Manipulating reaction enthalpies

In the previous section, we relied on a table of standard enthalpies of formation to compute enthalpy changes in general reactions. This enthalpy change ΔH_R° is related to the heat exchanged in the reaction. In this section, we will not use the tables of enthalpy anymore. Imagine you do not have access to this table. And we will find alternative ways to predict ΔH_f° given a series of reactions with known enthalpies. In short, you will have to identify the enthalpies that are zero—the enthalpies corresponding to an element in its natural state—and set up an equation that helps you find out the missing enthalpy.

Reverting reactions Imagine they give you the following reaction:



and you need to calculate the enthalpy change for this other reaction:

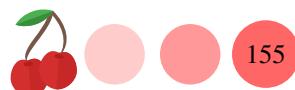


If you compare both reactions you will see the second reaction equals the first reaction but reverted. If you revert a reaction, the enthalpy change changes sign. Therefore, $\Delta H_2^\circ = 114 \text{ KJ}$.

Timing reactions by a number Imagine they give you the following reaction:

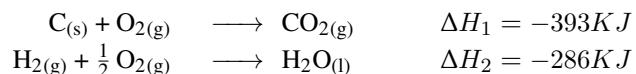


and you need to calculate the enthalpy change for this other reaction:

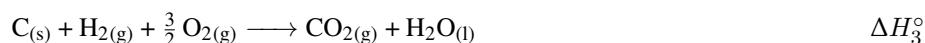


If you compare both reactions you will see the second reaction equals the first reaction time by two. If you time a reaction by two, the enthalpy change should also be timed by two. Therefore, $\Delta H_2^\circ = 2 \cdot -114 = -228 \text{ KJ}$.

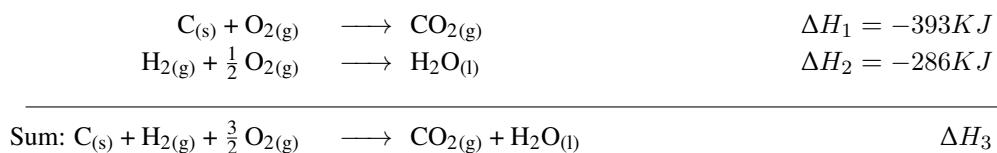
Combining reactions Imagine they give you the following two reactions:



and then ask the enthalpy change for the following reaction:



If you look closely at the last reaction, you will see it results from adding the first two reactions, so that:



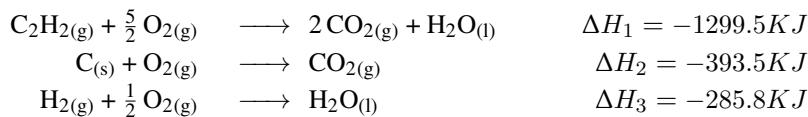
Therefore, $\Delta H_3 = \Delta H_1 + \Delta H_2 = -679 \text{ KJ}$. When adding two chemical reactions the resulting enthalpy is the result of adding the enthalpy of both reactions.

Sample Problem 83

Calculate the enthalpy for this reaction:



Given the following thermochemical equations:



SOLUTION

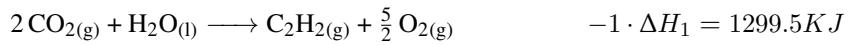
In order to get the enthalpy for reaction (4) we will have to combine reactions (1), (2) and (3), by adding, subtracting, or multiplying by a number so that the results adds up to reaction (4). A trick to do this is compare molecule by molecule in reaction (4) and see in which reaction we can find the same one. For example, reaction (4) contains $2\text{C}_{(\text{s})}$ in the reactant side. $\text{C}_{(\text{s})}$ can also be found in (2) also as reactant. However, in (2) $\text{C}_{(\text{s})}$ is not timed by 2. There we will use two times reaction (2):



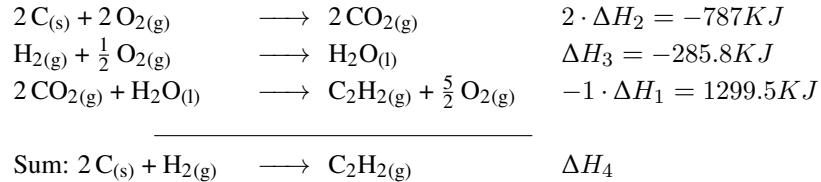
Reaction (4) also contains $\text{H}_{2(\text{g})}$, which can be found in (3). There we will use (3) as it is:



Reaction (4) also contains $\text{C}_2\text{H}_{2(\text{g})}$ as a product. We can find the same chemical in (1) but as a reactant. There we will have to invert (1):



If we add the three previous reactions, we have:

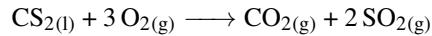


Therefore in the enthalpy for the reaction (4) will be:

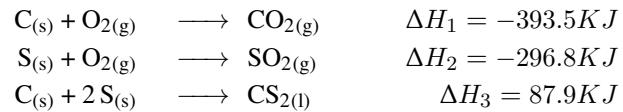
$$\Delta H_4^\circ = 2 \cdot \Delta H_2 + \Delta H_3 - 1 \cdot \Delta H_1 = 226.7 \text{KJ}$$

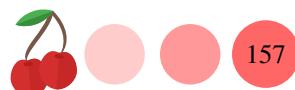
◆ STUDY CHECK

Calculate the enthalpy for this reaction:



Given the following thermochemical equations:



**Table 7.4 Standard enthalpy table at 1atm and 298K in KJ/mol.**

Substance	ΔH_f°	Substance	ΔH_f°	Substance	ΔH_f°
Aluminum					
$\text{Al}_{(s)}$	0	$\text{AlCl}_{3(s)}$	-705.63	$\text{Al}_2\text{O}_{3(s)}$	-1675.5
$\text{Al(OH)}_{3(s)}$	-1277	$\text{Al}_2(\text{SO}_4)_{3(s)}$	-3440	$\text{NH}_{3(aq)}$	-80.8
$\text{NH}_{3(g)}$	-46.1	$\text{NH}_4\text{NO}_{3(s)}$	-365.6	$\text{Al}_{(g)}$	314
Barium					
$\text{BaCl}_{2(s)}$	-858.6	$\text{BaCO}_{3(s)}$	-1213	$\text{Ba(OH)}_{2(s)}$	-944.7
$\text{BaO}_{(s)}$	-548.1	$\text{BaSO}_{4(s)}$	-1473.2	$\text{BaSO}_{4(s)}$	-1473.2
Boron					
$\text{BCl}_{3(s)}$	-402.96				
Bromine					
$\text{Br}_{2(l)}$	0	$\text{Br}^{-}_{(aq)}$	-121	$\text{Br}_{(g)}$	111.884
$\text{Br}_{2(g)}$	30.91	$\text{BrF}_{3(g)}$	-255.60	$\text{HBr}_{(g)}$	-36.29
Cadmium					
$\text{Cd}_{(s)}$	0	$\text{CdO}_{(s)}$	-258	$\text{Cd(OH)}_{2(s)}$	-561
$\text{CdS}_{(s)}$	-162	$\text{CdSO}_{4(s)}$	-935		
Calcium					
$\text{Ca}_{(s)}$	0	$\text{Ca}_{(g)}$	178.2	$\text{Ca}_{(g)}^{2+}$	1925.90
$\text{CaC}_{2(s)}$	-59.8	$\text{CaCO}_{3(s)}$	-1206.9	$\text{CaCl}_{2(s)}$	-795.8
$\text{CaCl}_{2(aq)}$	-877.3	$\text{Ca}_3(\text{PO}_4)_{2(s)}$	-4132	$\text{CaF}_{2(s)}$	-1219.6
$\text{CaH}_{2(s)}$	-186.2	$\text{Ca(OH)}_{2(s)}$	-986.09	$\text{Ca(OH)}_{2(aq)}$	-1002.82
$\text{CaO}_{(s)}$	-635.09	$\text{CaSO}_{4(s)}$	-1434.52	$\text{CaS}_{(s)}$	-482.4
$\text{CaSiO}_{3(s)}$	-1630				
Caesium					
$\text{Cs}_{(s)}$	0	$\text{Cs}_{(g)}$	76.50	$\text{Cs}_{(l)}$	2.09
$\text{Cs}_{(g)}^+$	457.964	$\text{CsCl}_{(s)}$	-443.04		
Carbon					
$\text{C}_{\text{graphite}(s)}$	0	$\text{C}_{\text{diamond}(s)}$	1.9	$\text{C}_{(g)}$	716.67
$\text{CO}_{2(g)}$	-393.509	$\text{CS}_{2(l)}$	89.41	$\text{CS}_{2(g)}$	116.7
$\text{CO}_{(g)}$	-110.525	$\text{COCl}_{2(g)}$	-218.8	$\text{CO}_{2(aq)}$	-419.26
$\text{HCO}_3^-_{(aq)}$	-689.93	$\text{CO}_3^{2-}_{(aq)}$	-675.23		
Chlorine					
$\text{Cl}_{(g)}$	121.7	$\text{Cl}^{-}_{(aq)}$	-167.2	$\text{Cl}_{2(g)}$	0
Chromium					
$\text{Cr}_{(s)}$	0				
Copper					
$\text{Cu}_{(s)}$	0	$\text{CuO}_{(s)}$	-155.2	$\text{CuSO}_{4(aq)}$	-769.98
Fluorine					
$\text{F}_{2(g)}$	0				
Hydrogen					
$\text{H}_{(g)}$	218	$\text{H}_{2(g)}$	0	$\text{H}_2\text{O}_{(g)}$	-241.818
$\text{H}_2\text{O}_{(l)}$	-285.8	$\text{H}^+_{(aq)}$	0	$\text{OH}^-_{(aq)}$	-230
H_2O_2	-187.8	$\text{H}_3\text{PO}_4_{(l)}$	-1288	$\text{HCN}_{(g)}$	130.5
$\text{HBr}_{(l)}$	-36.3	$\text{HCl}_{(g)}$	-92.30	$\text{HCl}_{(aq)}$	-167.2
$\text{HF}_{(g)}$	-273.3	$\text{HI}_{(g)}$	26.5		
Iodine					
$\text{I}_{2(s)}$	0	$\text{I}_{2(g)}$	62.438	$\text{I}_{2(aq)}$	23
$\text{I}^-_{(aq)}$	-55				



(cont.) Standard enthalpy table at 1atm and 298K.

Substance	ΔH_f°	Substance	ΔH_f°	Substance	ΔH_f°
Iron					
Fe _(s)	0	Fe ₃ C _(s)	5.4	FeCO _{3(s)}	-750.6
FeCl _{3(s)}	-399.4	FeO _(s)	-272	Fe ₃ O _{4(s)}	-1118.4
Fe ₂ O _{3(s)}	-824.2	FeSO _{4(s)}	-929	Fe ₂ (SO ₄) _{3(s)}	-2583
FeS _(s)	-102	FeS _{2(s)}	-178		
Lead					
Pb _(s)	0	PbO _{2(s)}	-277	PbS _(s)	-100
PbSO _{4(s)}	-920	Pb(NO ₃) _{2(s)}	-452	PbO _(s)	-276.6
Magnesium					
Mg _(s)	0	Mg ²⁺ _(aq)	-466.85	MgCO _{3(s)}	-1095.7
MgO _(s)	-601.6	MgSO _{4(s)}	-1278.2	MgCl _{2(s)}	-641.8
Manganese					
Mn _(s)	0	MnO _(s)	-384.9	MnO _{2(s)}	-519.7
Mn ₂ O _{3(s)}	-971	Mn ₃ O _{4(s)}	-1387	MnO _{4-(aq)}	-543
Mercury					
HgO _(s)	-90.83	HgS _(s)	-58.2		
Nitrogen					
N _{2(g)}	0	NH _{3(aq)}	-80.8	NH _{3(g)}	-45.90
NH ₄ Cl	-314.55	NO _{2(g)}	33.2	N ₂ O _(g)	82.05
NO _(g)	90.29	N ₂ O _{4(g)}	9.16	N ₂ O _{5(s)}	-43.1
Oxygen					
O _(g)	249	O _{2(g)}	0	O _{3(g)}	143
Phosphorus					
P _{4(s)}	0	P _{red(s)}	-17.4	P _{black(s)}	-39.3
PCl _{3(l)}	-319.7	PCl _{3(g)}	-278	PCl _{5(s)}	-440
PCl _{5(g)}	-321	P ₂ O _{5(s)}	-1505.5		
Potassium					
KBr _(s)	-392.2	K ₂ CO _{3(s)}	-1150	KClO _{3(s)}	-391.4
KCl _(s)	-436.68	KF _(s)	-562.6	K ₂ O _(s)	-363
KClO _{4(s)}	-430.12				
Silicon					
Si _(g)	368.2	SiC _(s)	-74.4	SiCl _{4(l)}	-640.1
SiO _{2(s)}	-910.86				
Silver					
AgBr _(s)	-99.5	AgCl _(s)	-127.01	AgI _(s)	-62.4
Ag ₂ O _(s)	-31.1	Ag ₂ S _(s)	-31.8		
Sodium					
Na _(s)	0	Na _(g)	+107.5	NaHCO _{3(s)}	-950.8
Na ₂ CO _{3(s)}	-1130.77	NaCl _(aq)	-407.27	NaCl _(s)	-411.12
NaF _(s)	-569.0	NaOH _(aq)	-469.15	NaOH _(s)	-425.93
Na ₂ O _(s)	-414.2				
Sulfur					
S ₈ monoclinic _(s)	0.3	S ₈ rhombic _(s)	0	H ₂ S _(g)	-20.63
SO _{2(g)}	-296.84	SO _{3(g)}	-395.7	H ₂ SO _{4(l)}	-814
Titanium					
Ti _(s)	0	Ti _(g)	468	TiCl _{4(g)}	-763.2
TiCl _{4(l)}	-804.2	TiO _{2(s)}	-944.7		
Zinc					
Zn _(g)	130.7	ZnCl _{2(s)}	-415.1	ZnO _(s)	-348.0



CHAPTER 7

ENERGY AND TEMPERATURE

7.1 Answer the following questions: (a) What is the name of the energy associated with the motion of particles in a substance? (b) What is the name of the energy stored in height?

7.2 Discuss the changes in potential and kinetic energy in the following scenarios: (a) When water falls down a waterfall (b) When a person throws away an object high up in the air

7.3 Indicate whether the following statement describes kinetic or potential energy: (a) Water on top of a waterfall (b) Hitting a wall with a hammer

7.4 Indicate whether the following statement describes kinetic or potential energy: (a) a car moving in the road (b) Water on the bottom of a waterfall

7.5 Carry the following conversions: (a) 100°C to K (b) 200°F to K (c) 500K to $^{\circ}\text{F}$

7.6 Carry the following conversions: (a) 20°C to $^{\circ}\text{F}$ (b) 300K to $^{\circ}\text{C}$ (c) 41°F to $^{\circ}\text{C}$

7.7 Carry the following conversions: (a) 100 Cal into kcal (b) 10000 cal into J (c) 4565J into Cal

7.8 Carry the following conversions: (a) 650J into calories (b) 50 kcal into Cal (c) 3.25 kcal into joules

FROM ENERGY TO TEMPERATURE

7.9 The same amount of heat is provided to a sample of two different metals, metal A ($c_e(A) = 0.3 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$) and metal B ($c_e(B) = 0.4 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$). Both samples have the same mass and are at the same temperature. Which metal A or B would reach a higher temperature?

7.10 The same amount of heat is provided to a sample of two different metals, metal A ($c_e(A) = 0.5 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$) and metal B ($c_e(B) = 0.4 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$). Both samples have the same mass and are at the same temperature. Which metal A or B would reach a higher temperature?

7.11 Two samples, A and B, have the same mass and are at the same temperature. If they are equally heated the final temperature of A is three times the one for B. Compare the specific heats of the samples.

7.12 Two samples, A and B, have the same mass and are at the same temperature. If they are equally heated the final temperature of B is two times the one for A. Compare the specific heats of the samples.

7.13 A 50g piece of aluminum ($c_e = 0.214 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$) initially at 25°C absorbs 100cal. Calculate the final temperature of the aluminum piece.

7.14 A 200g piece of iron ($c_e = 0.1 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$) initially at 15°C absorbs 1000cal. Calculate the final temperature of the metal piece.

7.15 How many calories are required to raise the temperature of a 35 g sample of iron from 25°C to 35°C ? Iron has a specific heat of $0.108 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$.

7.16 What is the final temperature of a 35 g sample of iron initially at 25°C after receiving 50cal? Iron has a specific heat of $0.108 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$.

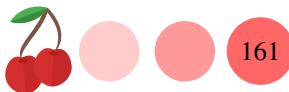
7.17 What is the initial temperature of a 50 g sample of aluminum that after receiving 50cal reaches a temperature of 50°C ? Al has a specific heat of $0.2 \frac{\text{cal}}{\text{g}^{\circ}\text{C}}$.

7.18 What is the specific heat of a metal if a 100 g sample at 25°C warms up until 50°C after receiving 100cal?

THE FIRST LAW OF THERMODYNAMICS

7.19 A sample of gas expands from 3 to 4 L at constant pressure. Using $1\text{L} \cdot \text{atm} = 101.3\text{J}$, calculate the work done in J under the following conditions: (a) The gas expands against the vacuum. (b) The gas expands against a constant pressure of 5atm

7.20 A sample of gas expands carrying out 120J of work to its surroundings while absorbing 150J of heat also from its surroundings. Calculate the change of the internal en-



ergy of the system in J.

CALORIMETRY

7.21 A 3 moles sample of C(s) is burned in a constant-volume calorimeter containing 40g of water. The temperature inside the calorimeter increases from 25.0°C to 25.89 °C. The calorimeter constant is 9.90 $\frac{kJ}{\circ C}$. Calculate the molar heat of the reaction.

7.22 A 10 grams sample of fructose (MW=180g/mol) is burned in a constant-volume calorimeter containing 50g of water. The temperature inside the calorimeter increases 7°C . The calorimeter constant is 10.8 $\frac{kJ}{\circ C}$. Calculate the molar heat of the reaction.

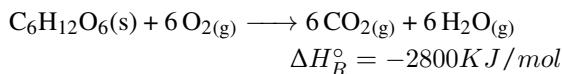
7.23 When a 0.09-g sample of trinitrotoluene (TNT, MW=213g/mol), is burned in a bomb calorimeter, the temperature increases from 23.5 °C to 27.1°C. The heat capacity of the calorimeter is 400 $\frac{J}{\circ C}$, and it contains 100 mL of water. Calculate the molar heat of the reaction. Remember that the density of water is 1g/mL.

7.24 We mix 50mL of 2M HCl with 100mL of 1.5M NaOH in a coffee-cup calorimeter. Both solutions are initially at 20°C. Calculate the final temperature of the solution in the calorimeter considering that the specific heat of the mixture is $4.184 \frac{J}{g \circ C}$ and the density of the solution is 1g/mL. The molar heat of the reaction is -56kJ/mol.

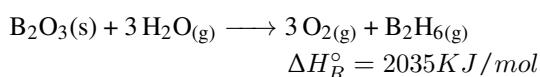
7.25 We mix 50mL of 2M HCl with 50mL of 2M NaOH in a coffee-cup calorimeter. Both solutions are initially at 40°C. Calculate the final temperature of the solution in the calorimeter considering that the specific heat of the mixture is $4.184 \frac{J}{g \circ C}$ and the density of the solution is 1g/mL. The molar heat of the reaction is -100kJ/mol.

REACTIONS AND ENERGY

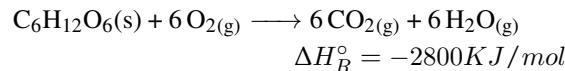
7.26 Identify the following reaction as endothermic or exothermic.



7.27 Identify the following reaction as endothermic or exothermic.



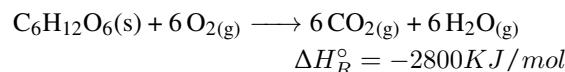
7.28 For the following reaction:



Fill the conversion factor:

$$\frac{\text{moles of O}_2}{-2800 \text{ KJ}}$$

7.29 In the following combustion reaction:



glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) burns to produce carbon dioxide and water. Calculate the heat involved in the combustion of 3 moles of glucose.

7.30 A potato contains 20 g of carbohydrate. If carbohydrate has a caloric value of 4 kcal/g, how many kcal are obtained from the carbohydrate in the potato?

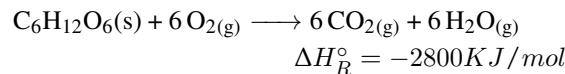
7.31 A diet has a total caloric intake of 1400 kcal. The diet consists of 50% carbohydrate, 35% protein, and 15% fat. The number of kcal of protein in the diet is

7.32 A serving of fish contains 50 g of protein and 4 g of fat. If protein has a caloric value of 4.0 kcal/g and fat has 9 kcal/g, how many kcal are in the serving?

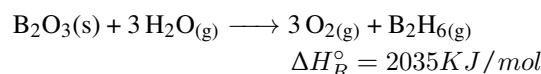
7.33 One large egg contains 6 g of protein and 6 g of fat. If protein has a caloric value of 4.0 kcal/g and fat has 9 kcal/g, how many kcal are in the egg?

REACTIONS AND ENERGY

7.34 Identify the following reaction as endothermic or exothermic.

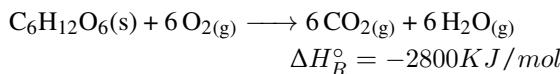


7.35 Identify the following reaction as endothermic or exothermic.





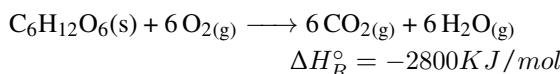
7.36 For the following reaction:



Fill the conversion factor:

$$\frac{\text{moles of O}_2}{-2800 \text{ KJ}}$$

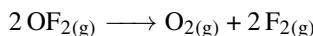
7.37 In the following combustion reaction:



glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) burns to produce carbon dioxide and water. Calculate the heat involved in the combustion of 3 moles of glucose.

ENTHALPY

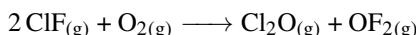
7.38 Calculate the enthalpy of reaction for:



given:

$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 24.5 \text{ KJ}$$

7.39 Calculate the enthalpy of reaction for:



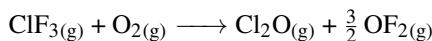
given:

$$\Delta H_f^\circ(\text{ClF}_{(\text{g})}) = -56 \text{ KJ}$$

$$\Delta H_f^\circ(\text{Cl}_2\text{O}_{(\text{g})}) = 88 \text{ KJ}$$

$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 25 \text{ KJ}$$

7.40 Calculate the enthalpy of reaction for:



given:

$$\Delta H_f^\circ(\text{ClF}_{3(\text{g})}) = -156 \text{ KJ}$$

$$\Delta H_f^\circ(\text{Cl}_2\text{O}_{(\text{g})}) = 88 \text{ KJ}$$

$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 25 \text{ KJ}$$

7.41 Calculate the enthalpy of reaction for:



given:

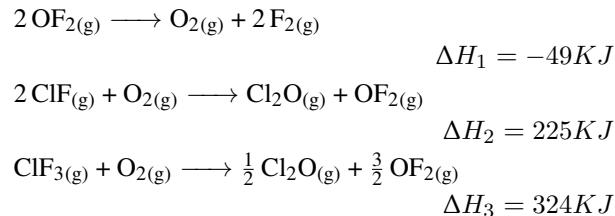
$$\Delta H_f^\circ(\text{CO}_{2(\text{g})}) = -393.5 \text{ KJ}$$

$$\Delta H_f^\circ(\text{H}_2\text{O}_{(\text{l})}) = -285.8 \text{ KJ}$$

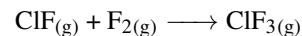
$$\Delta H_f^\circ(\text{C}_6\text{H}_{12}\text{O}_6(\text{s})) = -1273.3 \text{ KJ}$$

HESS'S LAW

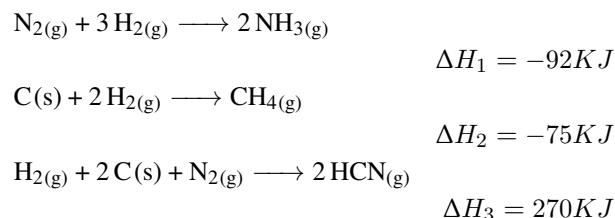
7.42 Using the following reactions:



Determine the enthalpy change for:



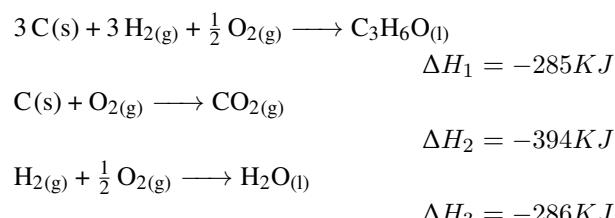
7.43 Using the following reactions:



Determine the enthalpy change for:



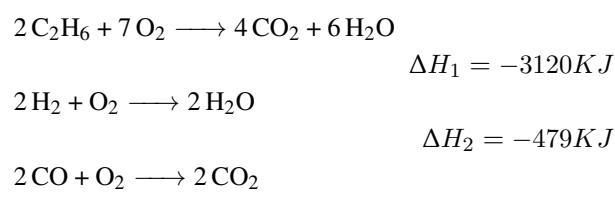
7.44 Using the following reactions:



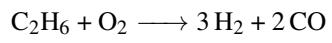
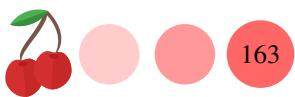
Determine the enthalpy change for:

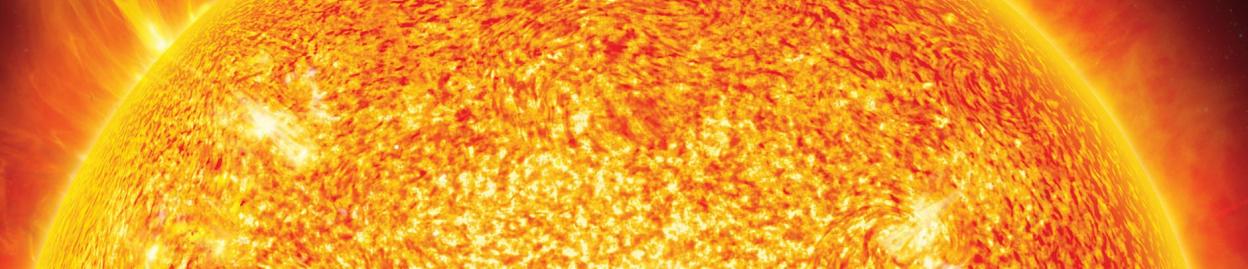


7.45 Using the following reactions:



Determine the enthalpy change for:





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Ch. 8. Electronic structure of atoms

MATTER is everywhere around you, from the water you drink to the air you inhale. The matter is made of elements and elements are made of atoms. In the world, we can also find light, that somehow at first sight seems different than matter. Light is warm and it has color. This chapter covers the structure of the atoms, with a focus on the structure of the many electrons that atoms are made of. It also focuses on light and the interaction of light with matter. You will be able to understand differences in electronic configuration.

“ The present is the only thing that has no end. ”
Schrödinger

8.1 The nature of light

Light—also called electromagnetic radiation—is a form of energy. When talking about light we normally refer to visible radiation. However, there are many different types of radiation. Think about the light coming from a bulb, the radiation that warms up your food in a microwave, or even when you warm up a pizza in the oven. This section will cover the properties of light.

Light as a wave Light behaves as a wave. Waves are characterized by their frequency, wavelength, and amplitude (see figure 8.1). The wavelength of a wave (λ , lambda) is the distance between identical points on successive waves (or successive peaks). The frequency of a wave (ν , nu) is the number of waves that pass through a particular point in one second. The amplitude (A) of a wave is the vertical distance from the zero to the top of the peak, or from the zero to the bottom of the peak. The amplitude of a wave is related to the intensity of the radiation. The speed of light through the vacuum is 3×10^8 m/s. However, the speed of light depends on the medium and light tends to slow down when traveling in a medium different than a vacuum.

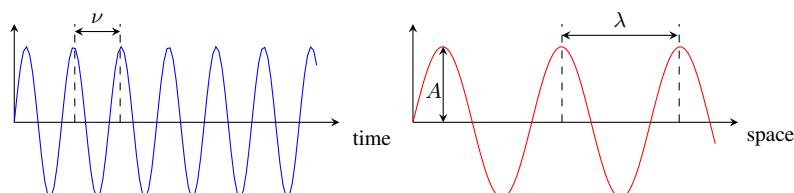


Figure 8.1 Properties of waves. Waves are characterized by its frequency, wavelength and amplitude and in the vacuum they travel at the speed of light.

The electromagnetic spectrum of light Visible light consists of electromagnetic waves, which have an electric field and magnetic field component (see Figure



8.2). These two components share the same wavelength, frequency, and speed but are perpendicular to each other.

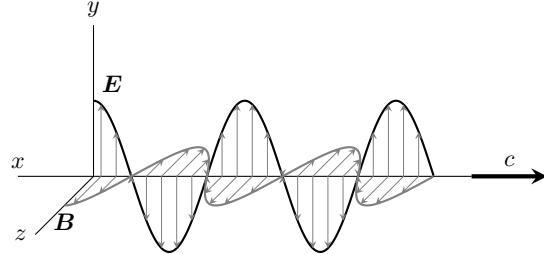


Figure 8.2 The electric (E) and magnetic (B) field components of an electromagnetic wave. Both fields are perpendicular.

The double-slit experiment: light diffraction The double-slit experiment was intended to demonstrate the wave nature of light. When a source of light passes through a narrow opening called a slit a bright spot is generated on the other side of the slit (see Figure 8.3). When a source of light passes through two slits surprising results arise. One would expect to see two bright spots, one per slit. However, what you really would see would be a series of bright spots and dark spots, resulting from the interference of light. As light is a wave it can interfere and light plus light does not always give more light, and can sometimes generate darkness. The bright spots result from the constructive interference of the light waves whereas the dark spots result from the destructive interference. Overall, waves propagate energy and the results of the propagation can be more light or less light depending on how these waves interfere.

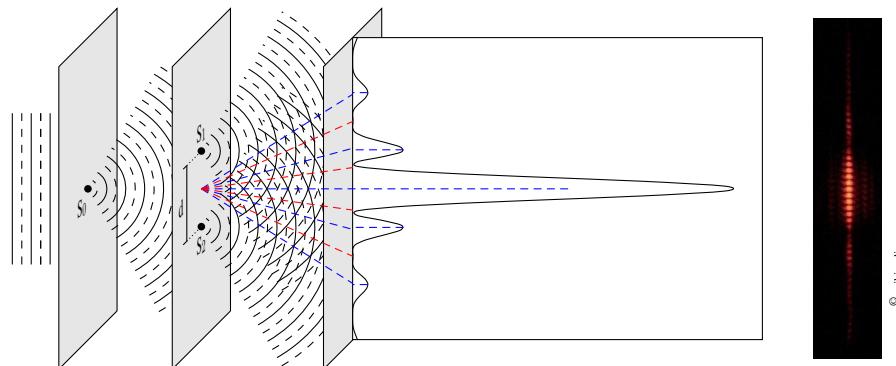


Figure 8.3 The double-slit experiment demonstrating the wave nature of light. Using one slit leads to a single bright spot. Using two slits leads to a set of patterns of light and darkness resulting from the interference of light. Red lines represent destructive interference whereas blue lines represent constructive interferences.

▼ Standing waves of a guitar



© wikipedia

▼ Traveling waves



© wikipedia

▼ Light is a wave



© PxHere

Types and color of radiation Depending on its frequency—or on its wavelength—radiation can be classified as gamma rays, x-rays, ultraviolet (UV), visible, infrared (IR), microwaves, or radio waves (see Table ?? and Figure 8.4). For example, radiation with a wavelength of 10^{-2} nm belongs to gamma rays radiation, whereas radiation with a wavelength of 10^4 nm belongs to the Infrared. Gamma rays are the most

energetic type of radiation, whereas radio waves are the less energetic waves. At the same time, radio waves have the largest wavelength. Light does not always have color. Only a small range of wavelengths belong to visible radiation and the visible spectrum corresponds to the set of visible frequencies. This means you will not be able to see, for example, IR radiation or gamma rays. The color of the radiation is also dependent on the wavelength—of the frequency as both are related—and for example $\lambda = 450 \text{ nm}$ will be blue light. Ultraviolet radiation is the most energetic visible radiation whereas infrared waves are the less energetic waves of the visible spectrum.

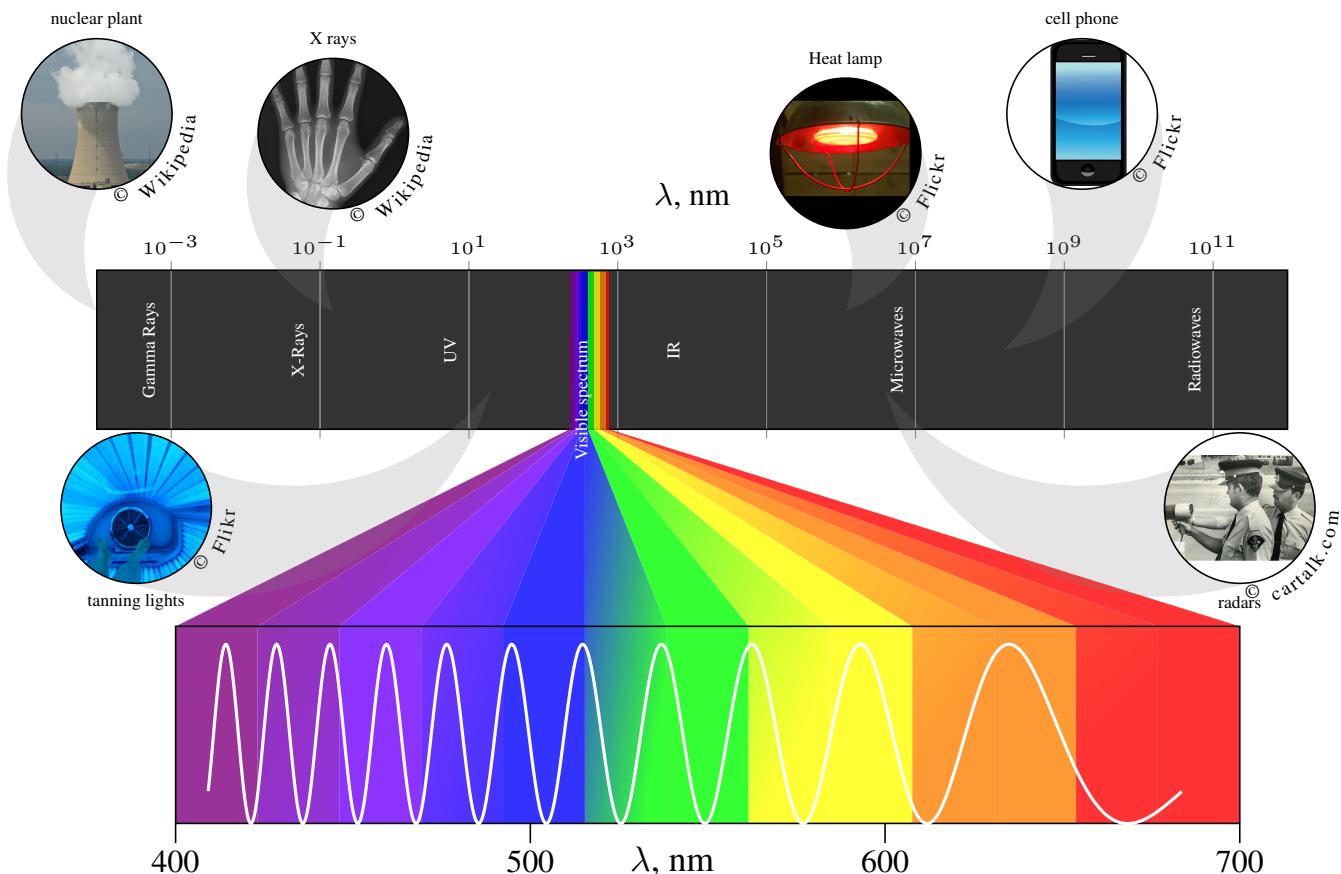


Figure 8.4 Spectrum of the electromagnetic radiation, from gamma rays (shortest wavelength) to radio waves (longest wavelength). The visible part of the spectrum ranges from 400 nm (violet) to 700 nm (red).

Sample Problem 84

Indicate: (a) the color of a radiation with $\lambda = 650 \text{ nm}$; (b) the type of a radiation with $\lambda = 10^5 \text{ nm}$.

SOLUTION

We can answer the first questions by inspecting the figure above we can see that $\lambda = 650 \text{ nm}$ corresponds to red radiation. To answer the second question we will also use the figure above, where we can see that $\lambda = 10^5 \text{ nm}$ belongs to the infrared.

❖ STUDY CHECK

Indicate: (a) the color of a radiation with $\nu = 400 \text{ nm}$; (b) the type of a radiation with $\nu = 10^{10} \text{ Hz}$.

**Table 8.6 Types and color of radiation**

Type of radiation	ν (Hz)	Color of radiation	λ (nm)
Gamma	$>3 \times 10^{19}$	Violet	380-450
X-rays	$3 \times 10^{19} - 3 \times 10^{16}$	Blue	450-485
UV	$3 \times 10^{16} - 8 \times 10^{14}$	Cyan	485-500
UV-visible	$4 \times 10^{14} - 8 \times 10^{14}$	Green	500-565
IR	$4 \times 10^{14} - 4 \times 10^{11}$	Yellow	565-590
MicroW	$3 \times 10^{11} - 3 \times 10^8$	Orange	590-625
RadioW	$3 \times 10^8 - 3 \times 10^3$	Red	625-740

8.2 Properties of light

Frequency and energy Light travels in time. That is the reason you can hear a whistle from afar. The *frequency* of radiation—the frequency of a specific type of light—characterizes how this radiation oscillates in time. The unit of frequency is the hertz and frequency are represented by the symbol ν . At the same time, frequency is connected to the energy of radiation. High-frequency radiation is very energetic. Think for example of gamma rays; these type of radiation produced in the nuclear plant has very high frequency and hence is very energetic. The formula that related frequency with energy is:

$$E = h\nu \quad \text{Frequency formula}$$

where:

E is the energy in joules

$h = 6.6 \times 10^{-34}$ is called Plank's constant

ν is frequency in hertz ($\text{Hz} = \text{s}^{-1}$)

As you can see in the previous formula, the frequency is directly proportional to the frequency. This equation has a historical character and was established by Max Plank in 1900. When a solid is warmed up to temperatures beyond 800K—this is called a black body—it emits radiation of different colors. The radiation emitted changes as the body are heated, and the light emitted goes from red to white. In the later part of the nineteenth century, experiments found that the amount of energy produced by a black body depends on the wavelength of the emitted radiation. However, none of the current theories (thermodynamics and classical physics) were able to explain that phenomenon. Plank came up with a solution to the dilemma. Classical physics assumes that radiant energy is continuous and radiation can be emitted and absorbed at any amount. To explain the blackbody radiation, Plank suggested that there is a minimum package of energy so that radiation could only be exchanged in discrete packages. The smallest amount of energy that can be emitted in the form of electromagnetic radiation was called *quantum* and equals $h\nu$, with h being Plank's constant. Based on his theory, the energy emitted by light can only be whole-number multiples of $h\nu$. This hypothesis was the key to solving the blackbody radiation dilemma and changing physics forever, marking the beginning of a new quantum theory.

The speed of light All light travel at the same speed in the vacuum and this speed is called the speed of light, c . The numerical value of the speed of light is 299 792 458 m / s which is close to 3×10^8 m/s. When light travels in a medium, like the water of



glass, its velocity can be lower than the speed of light as the medium slows down the propagation of light. At the same time, the speed of light is used to relate two properties of light: its frequency and its wavelength:

$$c = \nu \cdot \lambda \quad \text{the speed of light}$$

where:

c is the speed of light in the vacuum, 3×10^8 m/s

λ is wavelength in m

ν is the frequency in Hz.

If we want λ to be in nm we can use the following formula:

$$\nu = \frac{3 \times 10^{17}}{\lambda}$$

where:

ν is frequency in Hz

λ is wavelength in nm

$3 \times 10^{17} = c \cdot 10^9$ was adjusted to be able to use λ in nm

Mind that all radiation always travels at the speed of light in a vacuum. At the same time, this speed is the maximum speed allowed for any object, based on the principles of relativity.

Wavelength and energy Light also travels in space. As it moves, it oscillates in space. Think about dropping a stone into a lake. As you drop the pebble, the energy from the pebble propagates on the surface of the water. The energy of light also propagates in space and the *wavelength* of radiation is the distance between two consecutive peaks. As such, wavelength, represented by the letter λ and oftentimes with units of nm is also related to energy using the formula:

$$E = \frac{1.98 \times 10^{-16}}{\lambda} \quad \text{wavelength formula}$$

where:

E is the energy in joules

λ is wavelength in nm

$1.98 \times 10^{-16} = h \cdot c \cdot 10^9$ was adjusted to be able to use λ in nm

Mind that wavelength is inversely related to energy. That means, the larger wavelength the smaller energy. Also, mind that wavelength refers to the movement of light in space and frequency refers to the movement in time.

Sample Problem 85

Calculate: (a) the energy of a radiation with wavelength of 300nm; (b) the energy of a radiation with frequency of 10^{19} Hz; (c) the frequency of a radiation with wavelength of 300nm.

SOLUTION

(a) To answer the first question we will use the wavelength formula, as wave-



length is given ($\lambda = 300\text{nm}$) and we need to calculate the energy (E), in Joules:

$$E = \frac{1.98 \times 10^{-16}}{\lambda} = \frac{1.98 \times 10^{-16}}{300} = 6.6 \times 10^{-19}\text{J}$$

(b) To answer the second question we will use the frequency formula, as frequency is given ($\nu = 10^{19}\text{Hz}$) and we need to calculate the energy (E), in Joules:

$$E = 6.6 \times 10^{-34}\nu = 6.6 \times 10^{-34} \cdot 10^{19} = 6.6 \times 10^{-15}\text{J}$$

(c) To answer the last question we will use the formula that related frequency with wavelength—through the speed of light—as frequency is asked and wavelength is given ($\lambda = 300\text{nm}$); mind the units of frequency are hertz:

$$\nu = \frac{3 \times 10^{17}}{\lambda} = \frac{3 \times 10^{17}}{300} = 1 \times 10^{15}\text{Hz}$$

◆ STUDY CHECK

Calculate: (a) the wavelength of radiation with energy of $5.6 \times 10^{-19}\text{J}$; (b) the frequency of a radiation with frequency of $4.8 \times 10^{-18}\text{J}$; (c) the wavelength of a radiation with frequency of $2 \times 10^{15}\text{Hz}$.

8.3 The photoelectric effect

Sometimes, it is convenient to use another energy unit, called an electron volt, that makes these values more reasonable values.

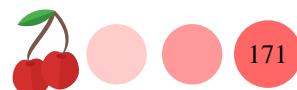
Table 8.6 Workfunctions and threshold frequencies

Element	W (eV)	ν_c , Hz
Ag	4.64	1.1×10^{15}
Ba	2.52	6.1×10^{14}
Fe	4.67	1.1×10^{15}
Al	4.20	1.0×10^{15}
Ca	2.87	6.9×10^{14}
Mn	4.1	9.9×10^{14}

$$1\text{eV} = 1.60218 \times 10^{-19}\text{J} \quad \text{or} \quad \frac{1\text{eV}}{1.60218 \times 10^{-19}\text{J}}$$

For example, the energy in eV of the first level is $E_1 = -13.6\text{eV}$, whereas the energy of the third level is $E_3 = -1.5\text{J}$.

The photoelectric effect The photoelectric effect was a mysterious phenomenon discovered early in the twentieth century. Scientists found that if you expose metals to light, under certain conditions, it emits electrons—it produced electricity (see Figure 8.5). They found that the intensity—the brightness—of the radiation was not a key component of this phenomenon, and not by increasing the intensity you were able to produce electrons. The key was the frequency of the radiation. For frequencies above a specific threshold radiation was produced. If the frequency was above that threshold—called threshold radiation, ν_c —then the larger the intensity of the radiation the more electrons were produced. At that time, the current theory of light, associating the intensity of light with energy, was unable to explain this phenomenon. Albert Einstein used Plank's theory of blackbody radiation to solve this mystery. He assumed that light is made of stream of particles called photons, each with a given energy, $h\nu$. The electrons of a metal are held by attractive forces. A property called work function W —or biding energy—tells how strongly the electrons of a metal are held together. In Table ?? you can find numerous work functions. Metals such as Fe have high workfunctions in comparison to metals such as Ca, which means it takes more energy to remove



an electron from the metal. Therefore, if the energy of the radiation was enough to overcome these forces, electron emission will happen. In other words, if $h\nu$ is larger than W the electron emission will happen, and the electrons emitted will have a kinetic energy (KE) equal to:

$$KE = 4.13 \times 10^{-15} \nu - W \quad \text{Photoelectric effect}$$

where:

KE is the kinetic energy of the emitted electrons in eV

4.13×10^{-15} is called Plank's constant in eV· s, h

ν is the frequency in hertz (Hz)

is the work function of the metal in eV

What is the threshold frequency, ν_c ? When the energy of the radiation is the same as the work function of the metal, then electrons are ejected. This way, the threshold frequency is just the work function of the metal converted in units of frequency:

$$\nu_c = \frac{W}{4.13 \times 10^{-15}} \quad \text{threshold frequency}$$

4.13×10^{-15} is called Plank's constant in eV· s, h , ν_c is the threshold frequency in hertz (Hz) and W is the workfunction of the metal in eV. Einstein's theory of the photoelectric effect shocked the scientific community. Before this theory, the light was considered a wave. Based on Einstein's theory, a wave poses properties of both a particle and a wave, and depending on the experiment one experiences light as a wave or as a particle.

Sample Problem 86

A metal with workfunction of 5eV is exposed to a radiation source with frequency of 2×10^{15} Hz. Indicate whether electrons will be ejected and if so, indicate the kinetic energy of these.

SOLUTION

Using the photoelectric effect equation we have that a radiation of 10^{15} Hz frequency has an energy of

$$4.13 \times 10^{-15} \cdot 2 \times 10^{15} = 8.27\text{eV}$$

As this values is larger than the workfunction of the metal ($W=5\text{eV}$), therefore electrons will be ejected with a kinetic energy of:

$$KE = 8.27 - 5 = 3.27\text{eV}$$

❖ STUDY CHECK

A metal with workfunction of 5eV is exposed to a radiation source with frequency of 9×10^{14} Hz. Indicate whether electrons will be ejected and if so, indicate the kinetic energy of these.

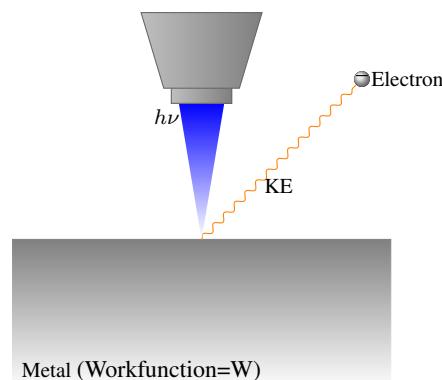


Figure 8.5 The photoelectric effect: when light with frequency (ν) larger than a threshold irradiates a metal, electrons are ejected with a specific kinetic energy (KE) that depends on the work function (W) of the metal.

8.4 The atomic line spectra

This section will explain the atomic spectra of atoms and in particular, hydrogen. Atoms emit light, but not any type of light as they emit specific frequencies of radiation. The atomic spectrum is a representation of the different wavelengths of the radiation emitted—or absorbed—by an atom. This section will gain insight into the reasons for the emission of specific frequencies of light and will introduce the Bohr model that justifies the lines in the atomic spectrum of hydrogen.

Spectrum of atoms The absorption spectrum of an atom is a representation of the different frequencies at which an atom absorbs or emits radiation. Each atom has a distinctive emission spectrum. Some of these lines correspond to the visible spectrum, that is, they can be seen. Others correspond to higher or lower parts of the spectrum. This section will cover the spectrum of hydrogen.

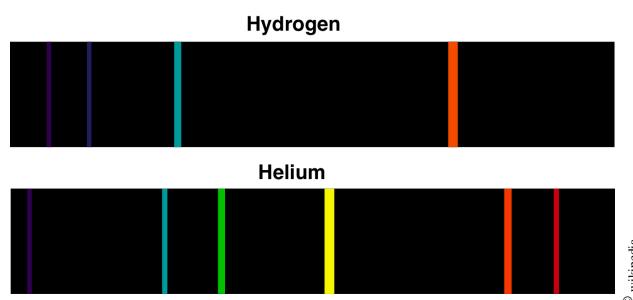


Figure 8.6 Atomic spectrum of two atoms showing the lines corresponding to the visible.

Atomic line spectrum of hydrogen Newton showed that sunlight (white light) is composed of various components of different colors. A similar type of radiation called emission spectra can be produced by heating a substance. Think for example of a hot piece of metal. Both the sun and a heated piece of metal have in common the fact that their spectrum is continuous and contains all wavelengths of visible light. We can achieve a similar effect by applying a high-voltage electrical discharge to a gas. The atomic line spectrum of a gas is a set of lines on a black (or sometimes white)

background (see Figure 8.6). These lines correspond to radiation emitted (or absorbed) by atoms. For the case of hydrogen (see Figure 8.7), some of these lines correspond to the visible spectrum, that is, have color—these are called the Balmer series. Other lines correspond to other parts of the spectra of radiation. This spectrum is historically important and was used to understand the structure of the electrons in the atom. In contrast to the sunlight spectrum, the atomic spectrum of a gas is not continuous but quantized.

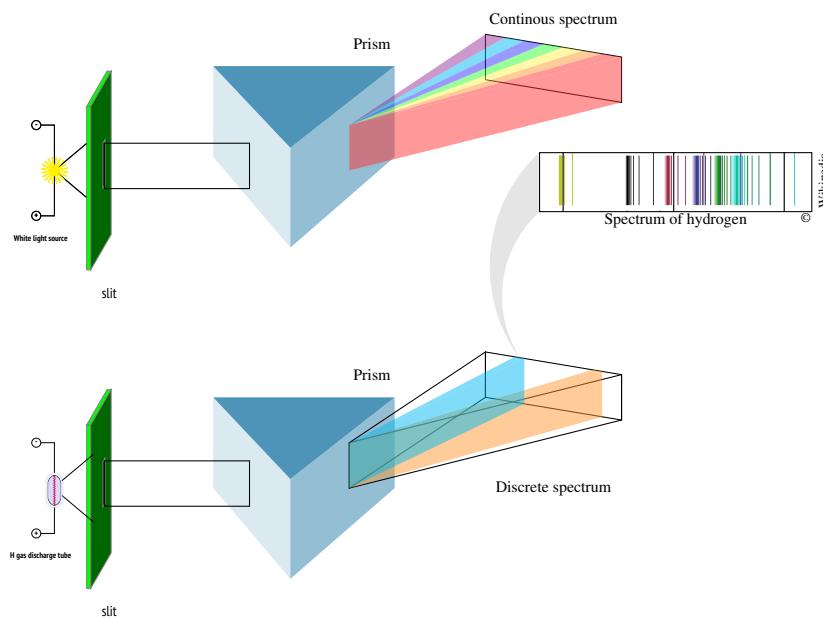


Figure 8.7 The spectrum of hydrogen: white light contains radiation of all colors of the visible spectrum whereas light coming from hydrogen contains a quantized series of lines.

8.5 Bohr's model

The Bohr model explains the electronic structure of hydrogen, in particular the spectrum of hydrogen and the position of the different energy lines. This model is based on the idea that the electron of hydrogen moves around the nucleus only in certain allowed circular orbits. Each orbit is called energy level, being characterized by an energy E_n and an integer number n . The following formula gives you the energy value for each level:

$$E_n = -2.178 \times 10^{-18} \frac{1}{n^2} \quad \text{Bohr formula in J}$$

where:

E_n is the energy of the level n in joules

n is the number of the level

$-2.178 \times 10^{-18} J = R_H$ is called the Rydberg constant ($-13.59 eV$)

For example, the energy of the first level is $E_1 = -2.178 \times 10^{-18} J$, whereas the energy of the third level is $E_3 = -5.44 \times 10^{-19} J$; the higher the n the larger—more positive—is the energy of the level.



Energy levels of hydrogen Let's gain deeper insight into the idea of an energy level. These are just numbers that represent the location—in energy units—of the different states that an electron can occupy in a hydrogen atom. The first level is E_1 and is the most negative energy value, being also the most stable level. In other words, the electrons in this level are tightly bonded to the nucleus. This energy level is called the fundamental energy level. The following levels (E_2, E_3, \dots, E_n) have more positive energy. For example, comparing E_2 and E_4 , we have that an electron on level number four ($E_4 = -0.85\text{eV}$) is less stable than on level two ($E_2 = -3.40\text{eV}$). Hence it would be easier to remove an electron from level number four than from level two. For small n values the levels are spread from each other. However, when n increases, the energy levels are closer and closer to each other. Electrons occupying energy levels with n higher than one are called excited states. Finally, there are an infinite number of levels and the highest energy (E_∞) level has an energy of 0J. The electron transitions between the different energy levels are what generate the emission spectrum of hydrogen (see Figure 8.8).

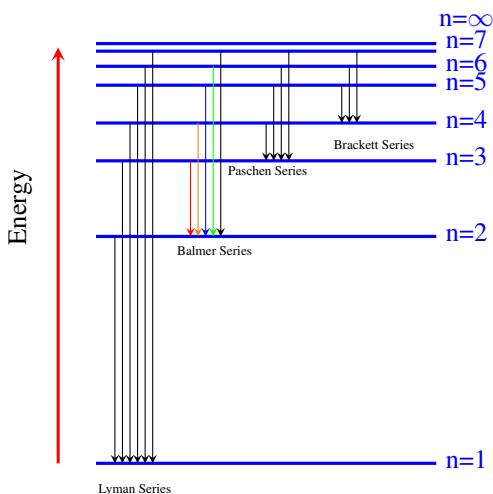


Figure 8.8 Energy levels of Hydrogen and the different emission series. Each series—called Lyman, Balmer, Paschen and Brackett—terminates at a different value of n .

Table 8.3 Emission spectrum of H

Series	n_f	n_i	Region
Lyman	1	2, 3, 4, ...	UV
Balmer	2	3, 4, 5, ...	Visible and UV
Paschen	3	4, 5, 6, ...	IR
Brackett	4	5, 6, 7, ...	IR

Transition energies Bohr's model can explain the atomic spectrum of hydrogen. Each line in the spectrum represents a transition between two levels of energy (see Figure 8.8). For example, the line at 102nm represents the transition of an electron between level three and level one, we call this $3 \rightarrow 1$. The atomic spectrum of hydrogen is obtained using exciting hydrogen atoms with energy so that the electron jumps from a lower level to a higher level. When the atom relaxes, it emits light as the electrons move back from high levels into lower—more stable—levels. This is called emission. The different possible emissions have names based on the person who discovered them (see Table 8.3). For example, the set of emissions that end up in the fundamental level ($n=1$) is called the Lyman series. Similarly, the set of emissions that end up in the level ($n=2$) is called the Balmer series. For example $3 \rightarrow 2$, $4 \rightarrow 2$, or $5 \rightarrow 2$. Only the Balmer series correspond to emissions on the visible spectra. The Lyman series belong to the ultraviolet and the Paschen and Brackett series belongs to the infrared.

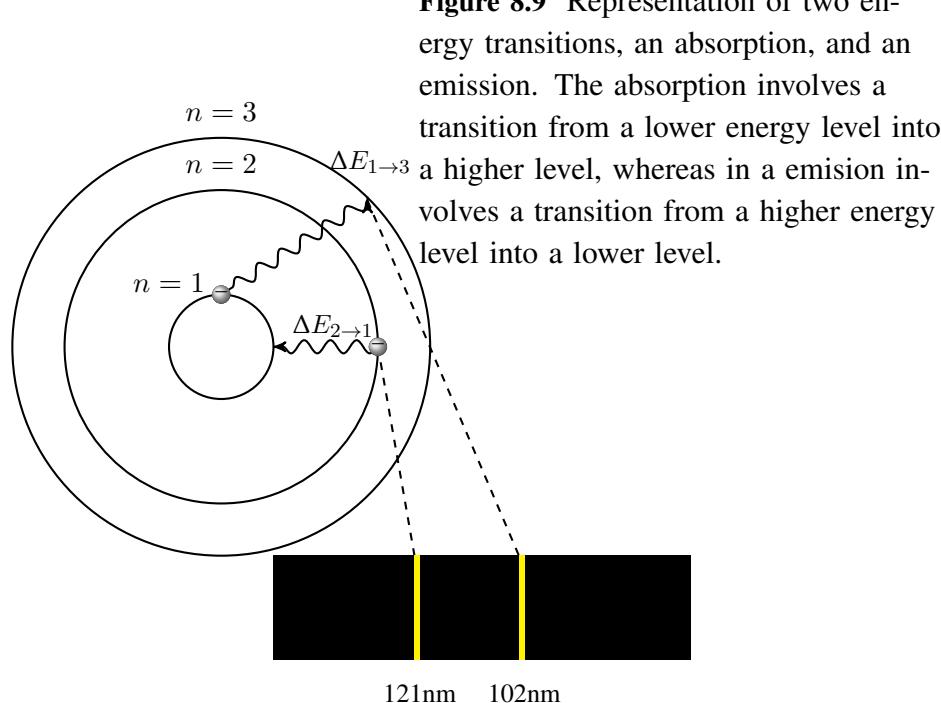


Figure 8.9 Representation of two energy transitions, an absorption, and an emission. The absorption involves a transition from a lower energy level into a higher level, whereas in an emission involves a transition from a higher energy level into a lower level.

Bohr's formula for energy transitions Bohr's formula gives you the values of the energy levels (see Figure 8.9). If we subtract the energy values for two energy levels, we obtain the energy for a transition. The energy for an electron transition between two energy levels, from n_1 to n_2 , is given by:

$$\Delta E_{n_1 \rightarrow n_2} = -2.178 \times 10^{-18} \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right)$$

Energy transition formula

where:

$\Delta E_{n_2 \rightarrow n_1}$ is the energy in joules for the transition, the line in the spectra

n_2 is the number of the final level

n_1 is the number of the initial level

$-2.178 \times 10^{-18} J = R_H$ is called the Rydberg ($-13.59 eV = R_H$)

Sample Problem 87

Calculate the following transition energies:

- $\Delta E_{4 \rightarrow 3}$ in J
- $\Delta E_{4 \rightarrow 3}$ in eV
- Calculate the final energy level for a transition with energy 1.34eV knowing the first energy level involved in the transition is $n = 3$

SOLUTION

- We will use the energy transition formula to calculate the energy needed to



move one electron from $n_1 = 4$ to $n_2 = 3$:

$$\begin{aligned}\Delta E_{n_2 \rightarrow n_1} &= -13.59 \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) = -13.59 \left(\frac{1}{3^2} - \frac{1}{4^2} \right) \\ &= -13.59 \left(0.111 - 0.0625 \right) = -0.66\text{eV}\end{aligned}$$

The transition energy is negative, this means the atom releases energy when transitioning between these two levels.

(b) We will use the energy transition formula this time in eV:

$$\begin{aligned}\Delta E_{n_2 \rightarrow n_1} &= -2.178 \times 10^{-18} \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) = -2.178 \times 10^{-18} \left(\frac{1}{3^2} - \frac{1}{4^2} \right) \\ &= -2.178 \times 10^{-18} \left(0.111 - 0.0625 \right) = -1.058 \times 10^{-19}\text{J}\end{aligned}$$

(c) In this case, we know $\Delta E_{n_2 \rightarrow 3}$ and we know the initial level is $n_1 = 3$. We can certainly solve for n_2 :

$$1.34 = -13.59 \left(\frac{1}{n_2^2} - \frac{1}{3^2} \right) = -13.59 \left(\frac{1}{n_2^2} - \frac{1}{9} \right)$$

Solving for n_2 we have: $n_2 = 9$. Mind you need to square root n_2^2 to get the final value of n_2 .

STUDY CHECK

Calculate the following transition energies: (a) $\Delta E_{9 \rightarrow 3}$ in J and (b) $\Delta E_{5 \rightarrow 4}$ in eV.

8.6 The wave properties of matter

Bohr's model was able to explain the experimental data for the hydrogen spectrum. Still, scientists—not even Bohr himself—did not know why electrons were restricted to moving in specific orbits. Louis de Broglie solved this question by suggesting that if light can behave—under some conditions—as a particle, perhaps particles such as electrons, can also behave as a wave—under certain circumstances (see Figure 8.10). De Broglie deduced that a particle and wave are related by the following expression:

$$\lambda = \frac{h}{m \cdot v}$$

where:

λ is De Broglie's wavelength of a particle

$6.6 \times 10^{-34}\text{Js}$ is called Plank's constant, h

$m \cdot v$ is the momentum of a particle, p , that depends on the mass and velocity of the particle

In general, the wavelength of a particle is referred to as the De Broglie wavelength and the mass associated with a wavelength is called the De Broglie mass. De Broglie came to this

conclusion using the following reasoning: if an electron in the hydrogen atoms behaves like a wave then its wavelength (λ) must fill the length of the circular orbit ($2\pi r$) so that

$$n\lambda = 2\pi r$$

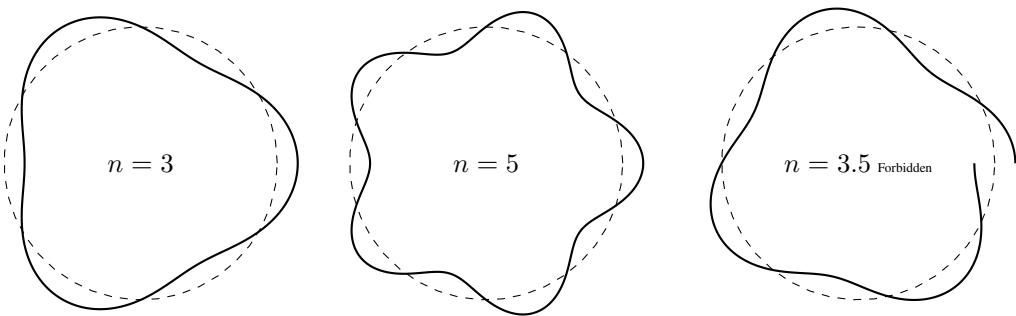


Figure 8.10 In the circular Bohr's orbits, electron could only have wavelengths that are a multiple of the orbit length, of the wave would cancel (forbidden orbits).

Sample Problem 88

Calculate the De Broglie wavelength of a tennis ball with mass 0.1Kg and velocity 100m/s.

SOLUTION

We will use De Broglie's relationship that associated a wavelength (λ) to a particle, in which the mass is 100g, the velocity 10m/s:

$$\lambda = \frac{6.6 \times 10^{-34} Js}{0.1 Kg \cdot 100 m/s} = 6.6 \times 10^{-35} m$$

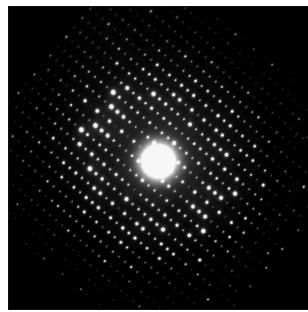
Regarding the units: remember J is Kgm^2/s^2 and therefore Js is the same as Kgm^2/s .

❖ STUDY CHECK

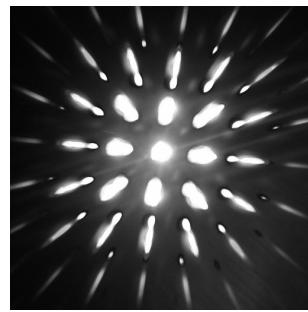
Calculate the De Broglie wavelength of an electron at a velocity of 100m/s given that an electron mass is $9 \times 10^{-31} \text{ kg}$.

Electron diffraction Following De Broglie's proposal that particles behave like waves under certain circumstances, particles, in particular, electrons were found to exhibit properties of a wave. The diffraction of electrons was achieved by Davidsson and Germer by directing a beam of electrons through a thin piece of gold foil creating a pattern similar to the diffraction of x-rays (see Figure 8.11).

▼Diffraction pattern of electrons ▼Diffraction pattern achieved with a laser



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Figure 8.11 Diffraction patterns produced by light and by matter

The uncertainty principle Waves result from the propagation of energy and



are not localized. Electrons behave as waves under certain conditions. To approach the problem of trying to locate a particle that behaves as a wave, the Heisenberg uncertainty principle states that it is impossible to measure simultaneously both the momentum ($m \cdot v$) and the position (x) of a particle. In other words, the uncertainty of the position (Δx) and the uncertainty on the momentum ($m \cdot \Delta v$) are linked by the relationship:

$$\Delta x \cdot m\Delta v \geq \frac{h}{4\pi} \quad (8.1)$$

This relation, involving Plank's constant h , should be interpreted as: if the uncertainty of the position is large, then the uncertainty of the velocity (or momentum) must be small. And the minimum values for the product of uncertainties if $\frac{h}{4\pi}$.

Sample Problem 89

The velocity of an electron is $2 \times 10^5 \pm 2 \times 10^3 \text{ m/s}$ given that the mass of an electron is $9 \times 10^{-31} \text{ kg}$. Calculate the minimum uncertainty in the position of the electron.

SOLUTION

We will use Heisenberg's relationship that links the uncertainty of the momentum and the position, given that the uncertainty of the velocity (Δv) is $2 \times 10^3 \text{ m/s}$ and h is $6.6 \times 10^{-34} \text{ kg m}^2/\text{s}$:

$$\Delta x \cdot 9 \times 10^{-31} \cdot 2 \times 10^3 \geq \frac{6.6 \times 10^{-34}}{4\pi}$$

We have that the uncertainty on the position Δx is larger or equal than $2.9 \times 10^{-8} \text{ m}$.

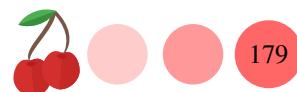
❖ STUDY CHECK

The uncertainty on the position of a particle with a mass of $1.7 \times 10^{-27} \text{ kg}$ is $\pm 10^{-11} \text{ m}$. Calculate the uncertainty on the velocity of the particle.

8.7 Quantum mechanics

Bohr's model was simplistic but still, it was able to correctly predict the fine structure of hydrogen—the atomic spectrum of hydrogen—and the energy transitions. The downside of this model resulted from considering that the electron moves in different orbits and that it did not provide a complete description of the behavior of the electrons in atoms. A correct assumption of the model was that the energy levels of the atom were quantized—electrons can only exist in specific energy levels characterized by the number n and not in a continuum of energy. This section will cover a more realistic theory that describes the structure of the atom: quantum mechanics. The outcomes of this section are the existence of orbitals and quantum numbers.

Quantized energy and continuum energy Quantum mechanics is a theory shared in physics and chemistry that describes the nature of matter. It is used to do modeling in chemistry—to model molecules and atoms. Think of an engineer designing a plane. Before building and selling the plane engineers carry out computer-based modeling to ensure the plane will work properly. Similarly, chemists carry out modeling to describe the properties of chemicals. The theory behind engineering modeling is classical mechanics, based on Newton's law. The theory behind chemistry modeling is



quantum mechanics, based on Schrödinger equation. Classical mechanics is based on the idea that the energy of a system, a plane or a car, is a continuum, that is, the car or a plane can have any possible energy, starting from zero to any number you can think of. Differently, quantum mechanics is based on the idea that the energy of a system, an atom or a molecule, is quantized, that is it can only be certain specific values.

The Schrödinger equation The Schrödinger equation is the fundamental equation in quantum mechanics. It was formulated by Erwin Schrödinger in 1926, an Austrian physicist, and it was based on complex mathematical techniques. This equation incorporates the electron behavior in terms of a particle through its mass and in terms of a wave through a wave-like function, Ψ .

$$\hat{H}\Psi = E\Psi$$

\hat{H} is called the hamiltonian operator and contains kinetic energy and potential energy component. Ψ , the wave function depends on the location of the space of each electron in the system. E are the energy levels. The solution of this equation required advanced calculus and will not be covered here. In contrast to the simple algebraic equation in which an answer is a simple number, the result of solving the Schrödinger equation is a set of functions and a number for each of these functions. The functions are called wavefunctions ($\{\Psi_1, \Psi_2, \dots, \Psi_n\}$), and for each wavefunction there is an energy value, leading to a set of energy levels ($\{E_1, E_2, \dots, E_n\}$). The introduction of The Schrödinger's equation mark the beginning of a new field in physics and chemistry called quantum mechanics or wave mechanics. Quantum mechanics do not allow us to specify the location of an electron in an atom, however, it allows us to identify the area in the space where the electron is most likely to be located at a given time. Electron density refers to the probability that an electron is found in a particular region of an atom.

The wave function: orbitals In quantum mechanics the wave function Ψ of an atom or a molecule (a system) is a complex function—it has an imaginary component—that contains all information of the system. Using this function, we can simulate the behavior of the system and extract its properties. You want to think of Ψ as a box that contains information, in particular all information of the system you want to simulate. When expressed in spherical coordinates, Ψ depends on the position (r) and two angles (θ and φ) of each electron of the system. This function Ψ *per se* has no real meaning or interpretation. Differently, Ψ^2 its square value has a real physical interpretation, representing the probability of finding an electron near a particular point in space. An orbital is a single-electron wave function. In other words, is a wave function that contains information about a single electron. The square value of an orbital represents the probability of finding an electron at a specific location. Electrons are very different than larger objects such as a tennis ball. Larger objects are localized, that is they are located at a specific point in space. Differently, electrons are delocalized, which means they are not located at a single point in space and time, and therefore we can only guess the probability of finding the electron at a specific point. Orbitals are mathematical functions with a radial and an angular component.

$$\Psi(r, \theta, \varphi) = \psi_n(r) \cdot Y_\ell^{m_\ell}(\theta, \varphi)$$

The radial part $\psi_n(r)$ describes how the orbital changes with the distance (r) along the space, whereas the angular part—these are called spherical harmonics, $Y_\ell^{m_\ell}$ —describes the symmetry of the orbital (see Figure 8.12). As a note, the term orbital is different



than the term orbit, which is used in classical physics to describe the trajectory of an object (e.g. a planet) and was used in Bohr's model to describe the different states of motion of the electrons in the hydrogen atom. When we say that an electron is located at a given orbital, we mean that the electron density distribution is described by the square of the wavefunction associated with that orbital.

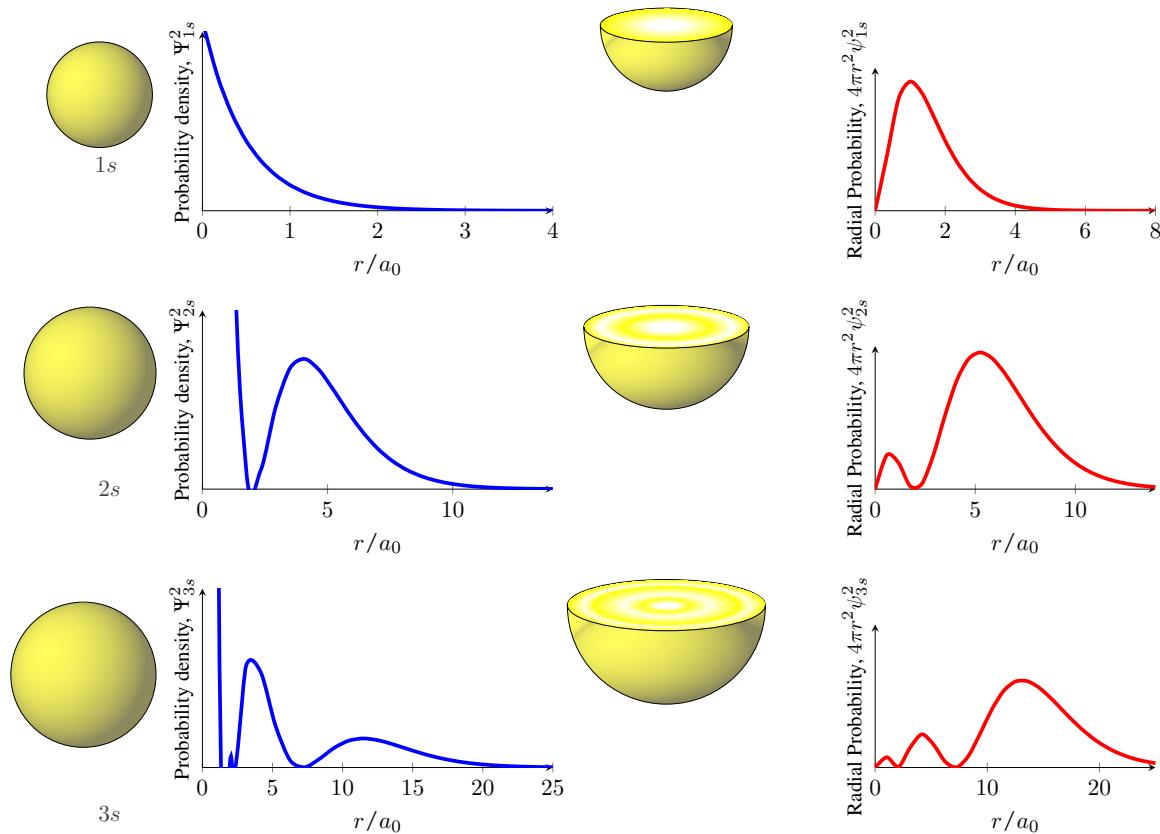


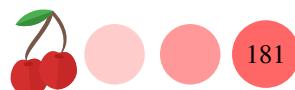
Figure 8.12 Three different representations of the s atomic orbitals of hydrogen: (left) boundary surface plots, (center) probability density plots (the orbital squared) with a sliced 3D surface plots, and (right) radial probability function. The value of a_0 , called Bohr's radius, is 52.9pm. The yellow circles inside the sliced 3D surface plots represent the orbital nodes.

8.8 Quantum numbers

In Bohr's model of the hydrogen atom, just a single number n was necessary to describe the electron state. Differently, in quantum mechanics, each orbital Ψ_{n,ℓ,m_ℓ} is characterized by three quantum numbers. These numbers differentiate each orbital from the rest. They are called: the principal quantum number n , the angular quantum number ℓ , and the magnetic quantum number m_ℓ . These quantum numbers are interrelated and not all combinations are allowed. We will describe this in the following, but just as an example, a possible combination would be $\Psi_{1,0,0}$ and $\Psi_{1,1,0}$ would be an impossible combination. Table 8.4 displays orbital labels and quantum number relationships. In the following, we will describe each quantum number separately.

Principal quantum number, n The principal quantum number n is related to the size of the orbital. The larger this value, the larger the orbital, and hence an electron in the orbital would have a greater average distance from the nucleus. n can only be integral values such as 1, 2, or 4 and it cannot be zero.

Angular quantum number, ℓ The second quantum number ℓ is called *angular*



quantum number and it describes the shape of the orbital. The values of ℓ are dictated by the value of n . In particular, ℓ goes from 0 until $n - 1$. For example, if $n = 3$, therefore ℓ can be: 0, 1 or 2. As such, n and ℓ can never be the same value, that is the reason why $\Psi_{1,1,0}$ does not represent a good orbital.

Magnetic quantum number, m_ℓ The third quantum number m_ℓ is called *magnetic quantum number* and is vaguely related to the orientation of the orbital. The values of m_ℓ depend on the value of ℓ . In general m_ℓ varies in a range of numbers including zero, $-l, -l-1, \dots, 0, \dots, l+1, l$. For example, if $\ell = 3$, m_ℓ can be any of these values: -3, -2, -1, 0, 1, 2, or 3. As a note, there is no relationship between the subindex labels (s, p, d or f) and the values of m_ℓ .

A fourth quantum number: the spin m_s Three quantum numbers are necessary to describe each orbital. Still, a fourth quantum number, the spin number m_s was necessary to understand why magnetic fields affect the emission spectra lines of hydrogen and sodium. m_s is called *spin quantum number* and can only be either $+1/2$ or $-1/2$.

The Pauli exclusion principle The Pauli exclusion principle states that there can not exist two electrons in an atom with the same values of the four quantum numbers. It tells that each electron is unique and it has to be differentiated with a unique combination of quantum numbers. Because of this, each orbital can only accommodate two different electrons, one with $-1/2$ spin and one with $+1/2$.

Radial distribution functions It is not straightforward to represent orbitals, as they extend throughout space. However, there are three common ways to represent s orbitals, and in general any orbital: (a) using the surface that contains 90% of the total electron probability, (b) using the orbital square, and (c) using the radial probability distribution. Let us elaborate on the meaning of radial probability distribution. Imagine the space is made of thin shells, like in the layers of an onion. By adding all shells we have the whole space. The radial probability distribution is the total probability of finding an electron in each shell which depends on the distance from the nucleus. The radial probability distribution is useful as the maximums on this function indicate the distances from the nucleus where it is most likely to find the electrons on a particular orbital. Among all radial distribution functions, the one for the $1s$ orbital also shows an interesting feature, and the distance from the nucleus where the probability of finding the electron is maximum $r = a_0$ is called Bohr's radius, 52.9pm.

Table 8.4 Orbital Labels (left side) and quantum number relationships (right side)

ℓ value	Orbital label	Quantum #	Values
0	s	n	1, 2, 3...
1	p	ℓ	0, 1, ..., $n-1$
2	d	m_ℓ	$-\ell, -\ell+1, \dots, 0, \dots, \ell-1, \ell$
3	f	m_s	$+1/2$ or $-1/2$

Sample Problem 90

Indicate if the following combination of quantum numbers is allowed:



<i>n</i>	<i>ℓ</i>	<i>m_ℓ</i>	<i>m_s</i>	Allowed?
1	1	0	+ $^1/2$	
2	0	0	+ $^1/2$	
3	3	-1	- $^1/2$	

SOLUTION

The four quantum numbers are not independent. The quantum number *n* is related to the quantum number *l* and the number *l* is related to *m_l*. The only quantum number that is independent is the spin, *m_s* which can be $+^1/2$ or $-^1/2$. The first combination is not possible, as if *n* = 1, *l* can only be *n* - 1, that is zero. The second combination is correct, as if *n* = 2, the number *l* can be: 0 or 1. At the same time if *l* = 0, then *m_l* can also be zero. And finally, the spin value of $+^1/2$ is allowed. The last combination is not allowed, as *n* and *l* cannot be the same number.

<i>n</i>	<i>ℓ</i>	<i>m_ℓ</i>	<i>m_s</i>	Allowed?
1	1	0	$+^1/2$	No
2	0	0	$+^1/2$	Yes
3	3	-1	$-^1/2$	No

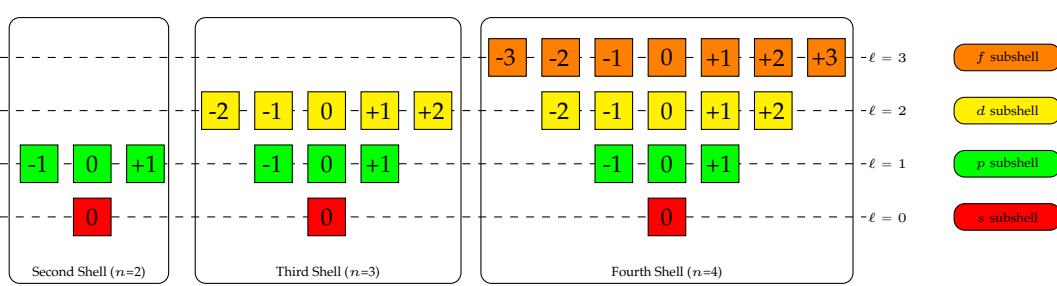
◆ STUDY CHECK

Indicate if the following combination of quantum numbers is allowed:

<i>n</i>	<i>ℓ</i>	<i>m_ℓ</i>	<i>m_s</i>	Allowed?
4	3	3	$+^1/2$	
4	3	3	0	
2	1	-1	$+^1/2$	

Shells and subshells (or levels and sublevels) A shell (or a level) is a collection of orbitals with the same value of *n* (see Figure ??). For example: $\Psi_{2,1,-1}$ and $\Psi_{2,0,1}$ belong to the same shell. A subshell (or sublevel) is a collection of orbitals with the same *n* and *l* values. For example: $\Psi_{2,1,-1}$ and $\Psi_{2,1,0}$ and $\Psi_{2,1,1}$ belong to the same subshell called *p*. The different subshells are names with the labels: *s*, *p*, *d*, and *f*.

Orbital labels: s, p, d and f There is a more convenient way to label orbitals than the Ψ_{n,ℓ,m_ℓ} notation. In this notation, *s* orbitals are orbitals with *l* = 0, whereas *p* orbitals have *l* = 1 and *d* orbitals have *l* = 2. Finally, *f* orbitals have *l* = 3. The principal quantum number should also be indicated before the label. For example, the orbitals $\Psi_{2,0,0}$ is a *2s* (Ψ_{2s}) and the orbital $\Psi_{2,1,-1}$ is a *2p*, that is Ψ_{2p} . The magnetic quantum number is not indicated in this notation. This is the most extended notation used to represent and refer to orbitals.



The shell and subshell distribution for different principal and angular quantum numbers. The same value of n belong to the same shell and orbitals with the same n and ℓ values are in the same subshell.

8.9 Atomic orbitals

The precise location of electrons in the atoms is unattainable. Differently, the electron location is described in terms of probability. An orbital is a three-dimensional area with the highest probability of finding an electron. Orbitals have different shapes and energy, as electrons in those have different stability. Some orbitals have a spherical shape, whereas others are lobular.

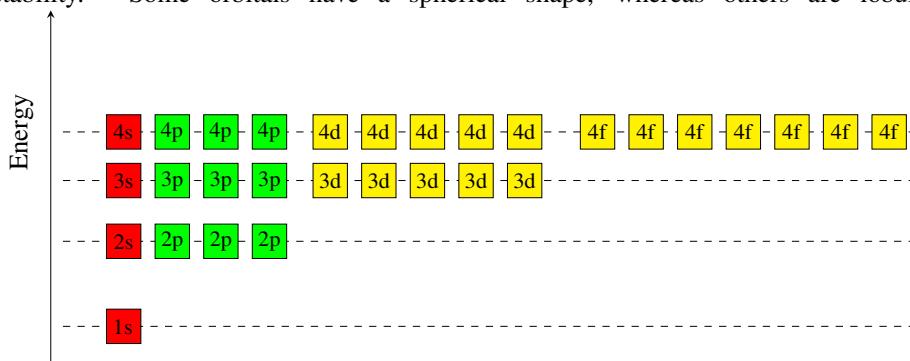


Figure 8.14 Energy of the different hydrogen orbitals. s orbitals have the lowest energy and hence are the most stable. Orbitals in the same shell ($2p$, $2s$) have the same energy. The larger the principal quantum number the more positive the energy, the less stable the orbital.

Energy levels In an atom, electrons are located at different levels. Each electron has a specific energy referred to as an *energy level* or energy shell (see Figure 8.14). This means that the energy of an electron is quantized, and it is not a continuous property: electrons can not have any energy value and can only have specific energy values. Electrons with the same energy are located at the same energy level. At the same time, some levels have lower energy and the electron in these levels are close to the nucleus being also strongly attached to it, whereas other levels have higher energy, and the electrons in these levels are less attached to the nucleus. Energy levels are labeled with a number n that equals a single number such as 1, 2, 3, and so on. The first energy level is $n = 1$ and never $n = 0$ —think of this as an apartment in a building, the first floor is flour one. For example, all electrons in level one $n = 1$ have the same energy. There is a limit to the number of electrons in an energy level and we call this occupancy. Only a few electrons can occupy the lower energy levels, while more electrons can be accommodated in higher energy levels. Level one can only fit two electrons, whereas level two can fit a total number of eight electrons. The maximum number of electrons



allowed in any energy level is calculated using the formula

$$2n^2 \quad (8.2)$$

in which n is the energy level. You can see by using this formula that for example, the third level can accommodate 18 electrons. Changes in energy levels imply energy exchange. For example, an electron absorbs energy when going from level 1 to level 2, and releases energy when going from level 3 to level 1. And the trend continues.

Sample Problem 91

How many electrons can you fit in the energy level $n=3$.

SOLUTION

We will use the formula $2n^2$ that gives the number of electrons that fit in a energy level n . As $n = 3$, we can fit 18 electrons in this level. Remember, the larger the energy level the more electrons we can fit.

◆ STUDY CHECK

At a given energy level you can fit 162 electrons. Identify the energy level.

Energy sublevels Each of the energy levels consists of one or more than one sublevel or subshell. The number of sublevels within a level equals the principal quantum number

$$n \quad (8.3)$$

being identified by a letter s , p , d , or f . For example, in level one we only have one sublevel called the s level, however, in level two we have two sublevels, the s , and p levels. In level three we have three sublevels, the s , the p , and the d levels. Finally, in level four we have four sublevels, the s , the p , the p , and the d levels.

Orbitals Sublevels contain orbitals. These are three-dimensional areas with the highest probability of finding electrons. s sublevels contain one orbital, p sublevels contain three orbitals, p sublevels contain three orbitals, d sublevels contain five orbitals and f sublevels contain seven orbitals. Each orbital can contain a maximum number of two electrons, each with a different property called spin. The orbitals in the s sublevel are called s orbitals. Orbitals in the p sublevel are called p orbitals, and so on.

s orbitals There is a single s subshell in every shell and each s subshell contains only a single orbital. For example, in the first energy level, there is a $1s$ orbital, whereas, in the second energy level, there is a $2s$ orbital. All s orbitals have an overall spherical shape with increasing size depending on the principal quantum number n (see Figure 8.15). For example, the $1s$ orbital is smaller than the $2s$, and so on.

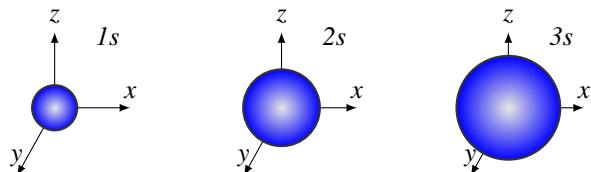


Figure 8.15 Surface plots of three s orbitals.

p orbitals There are three different p orbitals and each subshell with n larger than 2 has a p orbital. These three p orbitals are labeled p_x , p_y , and p_z , where the subindexes represent the direction of the axis along which each orbital is oriented. All three p

orbitals have the same size, shape, and energy. The larger the principal quantum number the larger the size of the orbital, and for example, a $3p_x$ is larger than a $2p_x$. The boundary surface diagrams of p orbitals expose their shape in the form of two lobes, and positive and one with a negative sign (see Figure 8.17).

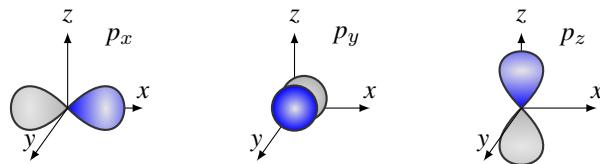


Figure 8.16 Surface plots of the three p orbitals.

d and f orbitals There are five d orbitals labeled as d_{xy} , d_{xz} , d_{yz} , d_{z^2} and $d_{x^2-y^2}$. The subindexes in the labels are related to the orientation of the orbital in space. None of the d_{xy} , d_{xz} , d_{yz} orbitals cross any of the axis, but d_{z^2} and $d_{x^2-y^2}$ do. In particular, the lobes of the d_{xy} orbitals are located in the xy plane, whereas $d_{x^2-y^2}$ cross the x and y axis and the d_{z^2} crosses the z axis. All five d orbitals have the same energy. These orbitals increase in size based on the principal quantum number and the $3d$ orbitals are smaller than $4d$. There are no d orbitals in the first or second shell. Regarding the f orbitals, there are seven orbitals with very complex shapes (see Figure 8.17).

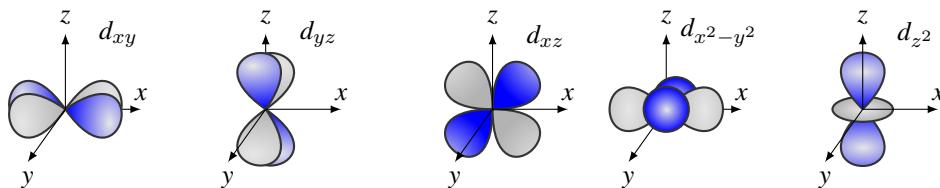


Figure 8.17 Surface plots of the three d orbitals.

8.10 Electronic configuration of an atom

Atoms have in general many electrons. These electrons are arranged in the atom in a very specific way creating what we know as an electronic structure. You want to think about the electronic configuration of an atom as a code that tells you the orbital location of each electron in the atom. There are two ways to present electronic configurations. One is called full electronic configuration (for example $1s^22s^1$) and the other one is called condensed electronic configuration (for example $[He]2s^1$). The full configuration displays all orbitals in an atom, whereas the abbreviated configuration only displays the valence electrons—these electrons are less-tied to the nucleus—and the noble gas core.

Orbital Filling: the aufbau principle Atoms in general contain numerous orbitals and each orbital should be filled with electrons. In every orbital, you can fill only a maximum number of electrons. For example, in a s orbital you can place a maximum of two electrons. That is why you will find s^1 orbitals and s^2 , with the latter being filled with electrons. In a p orbital you can place a maximum of six electrons and in a d orbital a maximum of ten. Finally, in a f orbital you can place fourteen or fewer electrons. For example, the orbital notation p^2 is correct as in p

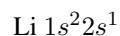


orbitals you can place six or fewer electrons. In this case, this orbital still has space to accept more electrons. Differently, the notation d^{12} is incorrect, as in d orbitals you can fit ten or fewer electrons and never twelve. The Aufbau (build up) principle states that the electronic configuration of an atom can be obtained by adding one by one all electrons in the element. In order to fill the orbitals you should follow Figure 8.18. You start from the top of the table and follow the arrows that indicate the orbitals ordering. For example, the first orbital to be filled will be $1s$. After that, you should fill in $2s$ and $2p$. After that you should fill $3s$, $3p$, $4s$, $3d$, and $4p$. There is a maximum number of electrons that can occupy each orbital. An s orbital holds a maximum of 2 electrons. A p orbital takes up to 6 electrons, a d orbital can hold up to 10 electrons, and an f orbital holds a maximum of 14 electrons. An orbital can be completely filled with electrons, partially filled, or empty. For example, a $3s^1$ is half-filled with one electron and $2p^6$ is completely filled. Another example, a $3d$ orbital is empty and can accommodate a maximum of 10 electrons.

Full electron Configuration The full electron configuration of an atom is obtained by placing the total number of electrons of the atom in different orbitals with increasing energy. For example, the electron configuration for helium is written as



and the one for Li is



First, how do we know the total number of electrons in an atom? That is the same as the atomic number and is indicated in the periodic table. Look for the element and the atomic number is on the top left side of the element. For example, the atomic number of hydrogen is one, and the number of electrons in He is two. Similarly, nitrogen has seven electrons. Second, how do we know which orbitals need to be filled? Figure 8.19 shows the orbital order. You need to start from the top of the image, from orbital $1s$, and proceed to the next arrow, starting from the end of the arrow. This way, after $1s$ goes $2s$ and then $2p$, $3s$, $3p$, $4s$, and $3d$. Mind that every s orbital can only fit two electrons, and p orbitals can fit six electrons, and so on. The following example will help you construct the electron configuration for a given atom.

Sample Problem 92

Obtain the full electronic configuration of C.

SOLUTION

The atomic number of C is $Z=6$ and that means C has 6 electrons. The orbital order from Figure ?? is: $1s, 2s, 2p, 3s$, etc. Each s orbital can fit two electrons, whereas the occupancy of the p orbitals is six electrons. Hence the electronic configuration of C is: $1s^2 2s^2 2p^2$. The s orbitals are all filled, whereas the p orbital is only occupied with two electrons.

❖ STUDY CHECK

Obtain the full electronic configuration of Ni.

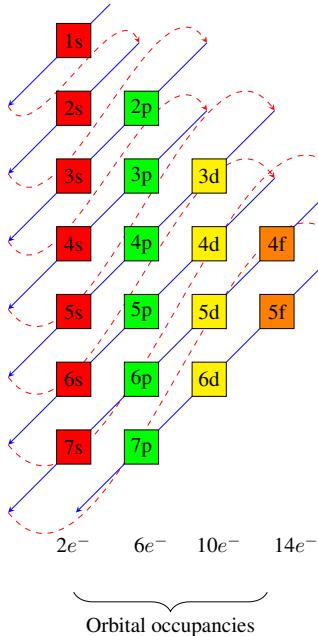
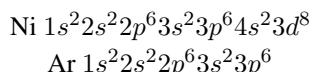
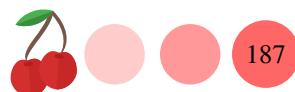


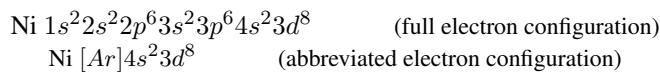
Figure 8.19 Orbital filling order.

Abbreviated Electron Configuration and orbital diagrams Let us compare the electronic configuration of Ni and Ar. We have:





We call this configuration the *full electronic configuration*. If you look carefully, you will see that both configurations resemble, and in particular, the configuration of Ni is the same as the configuration of Ar with two extra orbitals added. We say Ni has the core of Ar and 10 electrons on its valence. We can represent this fact by indicating Ar with brackets:



The orbital diagrams are boxed diagrams indicating the valence electrons such as:



We call this last configuration the *abbreviated electronic configuration*. You can figure out faster the abbreviated electronic configuration by looking for the noble gas on the table on the row above the element, and the period (row on the table) of the element. Ni is located in period number four and the noble gas above this period is Ar. At the same time, Ar has 18 electrons. That will give you the core $[\text{Ar}]$ with 18 electrons, and the remaining 10 electrons (Ni has 28 electrons) starting with the orbital $4s$, according to period four. The electrons in the noble gas core are called *core electrons*, whereas the rest of the electrons are known as *valence electrons*. For the case of Ni, we have that it has 18 core electrons in the Ar core and 10 electrons in the valence. Let us work on another example: Cd. It has 48 electrons and is located in group 5. The noble gas in the group above is Kr with 36 electrons. The core will be Kr—the noble gas on the period above—and we start right away filling $5s$ electrons—Cd belongs to period five. In the valence electrons, we will place 12 electrons. Hence, the abbreviated configuration will be $[\text{Kr}]5s^2 4d^{10}$.

Sample Problem 93

Obtain the full and abbreviated electronic configuration of Silver (Ag, Z=47) using the fact that the 4d and 5s orbitals switch order, being the d orbital filled first.

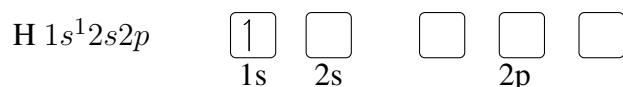
SOLUTION

The atomic number of Ag is Z=47 and that means Ag has 47 electrons. The orbital order is: 1s, 2s, 2p, 3s, etc. Each s orbital can fit two electrons, whereas the occupancy of the p orbitals is six electrons, and d orbitals can fit 10 electrons. We will use the fact that the 4d orbital fills before the 5s. Hence the full electronic configuration of Ag is: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^1$. As Kr is the noble gas on top with 36 electrons, the abbreviated electronic configuration of Ag is: $[\text{Kr}]4d^{10} 5s^1$. Ag has 36 core electrons and 11 valence electrons.

❖ STUDY CHECK

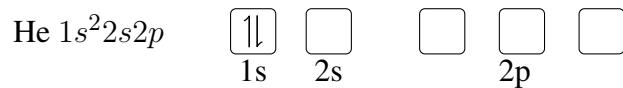
Obtain the abbreviated electronic configuration of Cobalt (Co, Z=27).

Hund's rule Let us build up the electron configuration of a series of atoms. Starting with hydrogen, with one electron, we have that only the 1s orbitals will be filled:

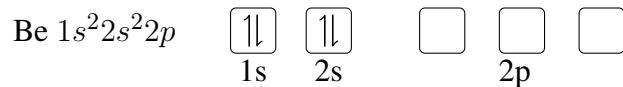
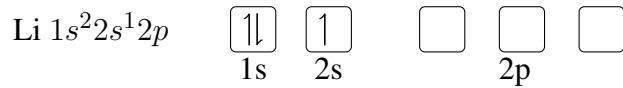




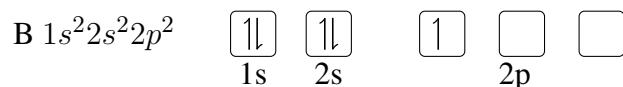
For the case of helium, with two electrons, we have that based on Pauli's principle both electrons have different quantum numbers and to differentiate this we will represent the pair of electrons with arrows in opposite directions. We say both electrons are paired:



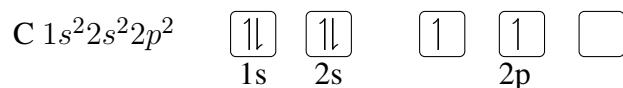
Now, in the case of Lithium and Beryllium, we have a similar situation. Lithium has a single unpaired electron and Beryllium has a set of paired electrons in the $2s$ orbital:



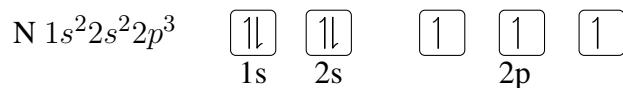
The next element, Boron, has one electron in a p orbital. As all p orbitals are degenerate—they have the same energy—we can place that single electron in any of the p orbitals. Normally, we use the one on the left:



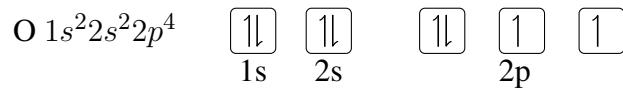
For the case of Carbon, as we need to place two electrons in the p orbitals, Hund's rule states that we need to place the electron maximizing the number of unpaired electrons. In other words, the second electron goes into a separate p orbital, just like below:



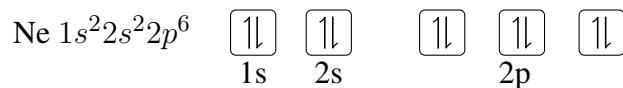
Similarly, in the case of Nitrogen, we have:

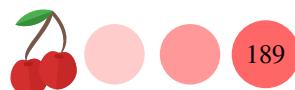


Now, for the case of oxygen, as we cannot place that extra electron in a separate p orbital we have to start pairing electrons:



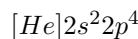
Finally, in the case of Neon, we have the whole second shell filled with electrons:



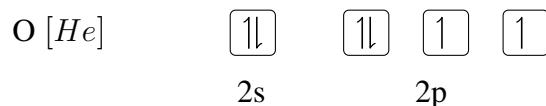


Sample Problem 94

Obtain the orbital diagram for oxygen given the electron configuration:

**SOLUTION**

The orbital diagram should include an s and a p sublevel. The *s* sublevel contains a single orbital represented by a box, whereas the *p* sublevel contain three different orbitals, and three boxes. The *s* orbital is fully occupied with two electrons, whereas the *p* sublevel contain only four electrons. The first three *p* electron will occupy separate boxes while the fourth electron will occupy the first box with opposite spin.

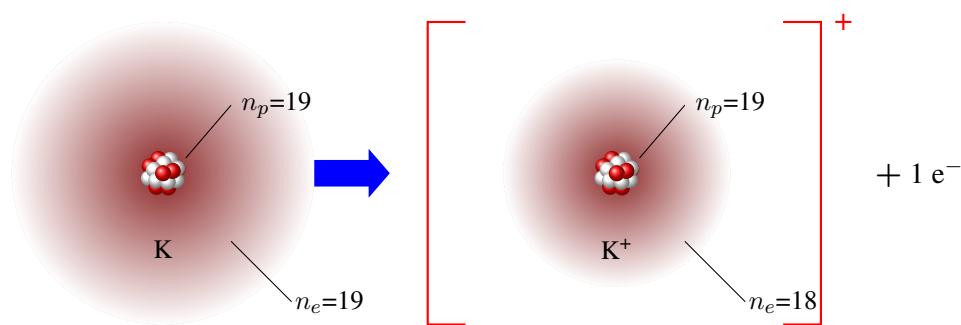
**◆ STUDY CHECK**

Obtain the orbital diagram for Li given the electron configuration: $[He]2s^1$.

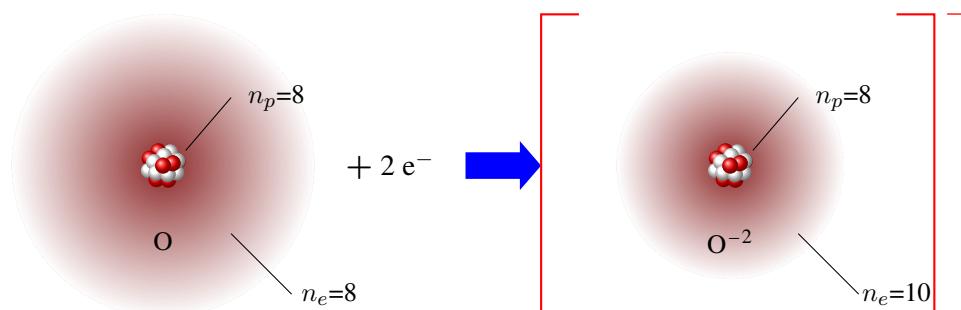
8.11 Monoatomic ions: cations and anions

Most chemical elements are found in nature combined with other elements, forming compounds. An exception is the noble gases which only combine with other elements under very extreme conditions. The reason for the stability of noble gases—their inability to form compounds—result from their electronic configuration: all noble gases have a valence shell filled with electrons, without empty orbitals. Elements combine through an electron exchange process; they receive or gain electron density, or simply electrons, to achieve a stable electron configuration. In other words, they exchange electrons to acquire an octet of eight valence electrons. Ions are atoms with an electrical charge that result from the process of gaining or losing electrons so that atoms reach a stable electron configuration.

Cations Elements from groups 1A, 2A, and 3A have low ionization energy and hence can easily lose their valence electrons forming cations (pronounced cat-eye-uns). For example, Potassium located in group 1A with electron configuration $[Ar] 4s^1$ can readily lose its only valence electron reaching the electron configuration of its core, Ar (see Figure 8.20). When losing a negatively charged electron as the number of protons in the atom does not change, it acquires a positive ionic charge of +1. When a cation is formed the atomic radius, indeed the ionic radius also changes becoming smaller, as cations result from the loss of electron density. Ca with electron configuration $[Ar] 4s^2$ and located in the group 2S loses two electrons reaching the electron configuration of Ar, its noble gas core, and the ionic charge of Ca is +2.

**Figure 8.20** The formation of a potassium cation

Anions Elements from groups 4A, 5A, and 6A have high ionization energy and hence can easily gain valence electrons forming anions (pronounced an-eye-uns). For example, F located in group 7A with electron configuration [He] $2s^2 2p^5$ can readily gain one valence electron reaching the electron configuration of Ne (see Figure 8.21). When gaining a negatively charged electron as the number of protons in the atom does not change, it acquires a negative ionic charge of -1 . Similarly, O located in group 6A with electron configuration [He] $2s^2 2p^4$ can readily gain two valence electrons reaching the electron configuration of Ne. When gaining two negatively charged electrons, it acquires two negative ionic charges -2 .

**Figure 8.21** The formation of an oxygen anion.**Table 8.6** Ionic charges from group numbers

Nobel Gas		Group 1A	Group 2A	Group 3A	Group 5A	Group 6A	Group 7A		Nobel Gas
He		Li^+							Ne
Ne		Na^+	Mg^{2+}	Al^{3+}	N^{3-}	O^{2-}	F^-		Ar
Ar		K^+	Ca^{2+}		P^{3-}	S^{2-}	Cl^-		Kr
Kr		Rb^+	Se^{+2}			Br^-			Xe
Xe		Cs^+	Ba^{+2}			I^-			



Ionic charges from group numbers Most of the representative elements lose or gain electrons to achieve the electronic configuration of the nearest noble gas. Therefore, one can obtain the ionic charges based on the group numbers. Elements belonging to Group 1A have an atomic charge of 1+ and they will lose one electron to reach the corresponding noble gas electronic configuration. For example, the ionic charge of Li is 1+. Mind we write 1+ and not +1. The same is for groups 2A and 3A with ionic charges of 2+ and 3+, respectively. Elements belonging to Group 7A have an atomic charge of -1 and they will gain one electron to reach the corresponding noble gas electronic configuration. Same for groups 6A and 5A with ionic charges of 2- and 3-, respectively. Elements in group 4A do not typically form ions and hence do not have an ionic charge. Table ?? gives different ionic charges obtained from group numbers.



8.12 Periodic Trends

Some atomic properties are periodic, which means that they follow certain trends in the periodic table. These properties increase or decrease across a period and then the trend is repeated in each successive period or group. We will consider here five atomic properties: the effective charge, atomic (or ionic) size, the ionization energy, the metallic character, and the electronegativity. Figure 8.25 summarizes the different periodic trends across the periodic table.

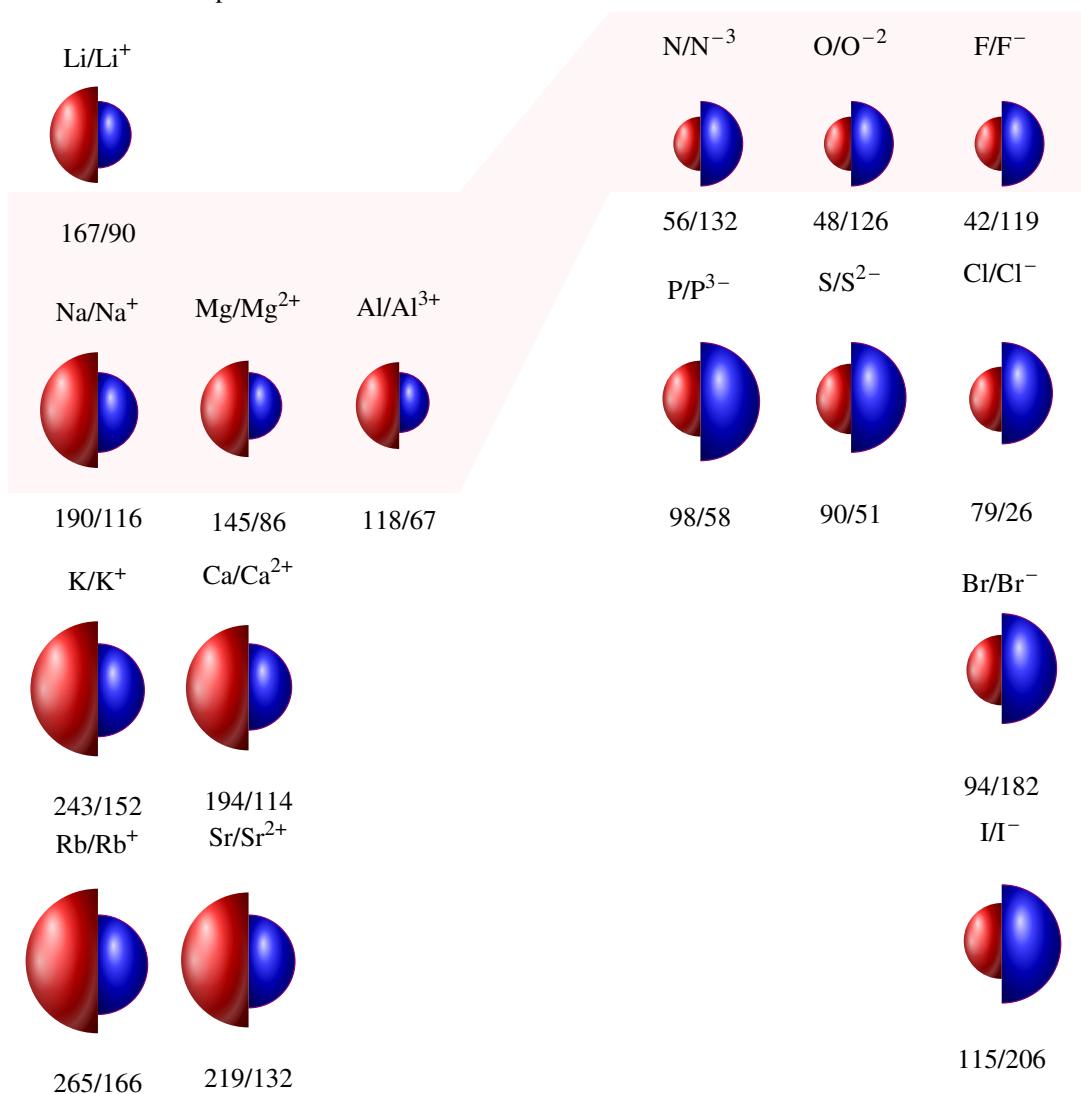


Figure 8.22 Ionic and atomic radius in pm across the periodic table

Effective charge The nuclear charge (Z) of an atom is the number of protons in the nucleus. In atoms with more than one electron, each electron is exposed to a nuclear effective charge (Z_{eff}) as the electrons partially compensate for the nuclear charge creating an effective nuclear charge. This way, the effective nuclear charge is the actual magnitude of the positive charge experienced by an electron. In atoms with many electrons, an electron is partially shielded from the positive charge of the nucleus. Among the different types of electrons in an atom (valence and core), core electrons are more effective at shielding, and as such Z_{eff} increases from left to right across the periodic table. As the number of core electrons remains the same and the atomic number increases from left to right across the table, Z_{eff} follows this trend too. The

effective nuclear charge is given by

$$Z_{eff} = Z - \sigma$$

where σ is the shielding constant.

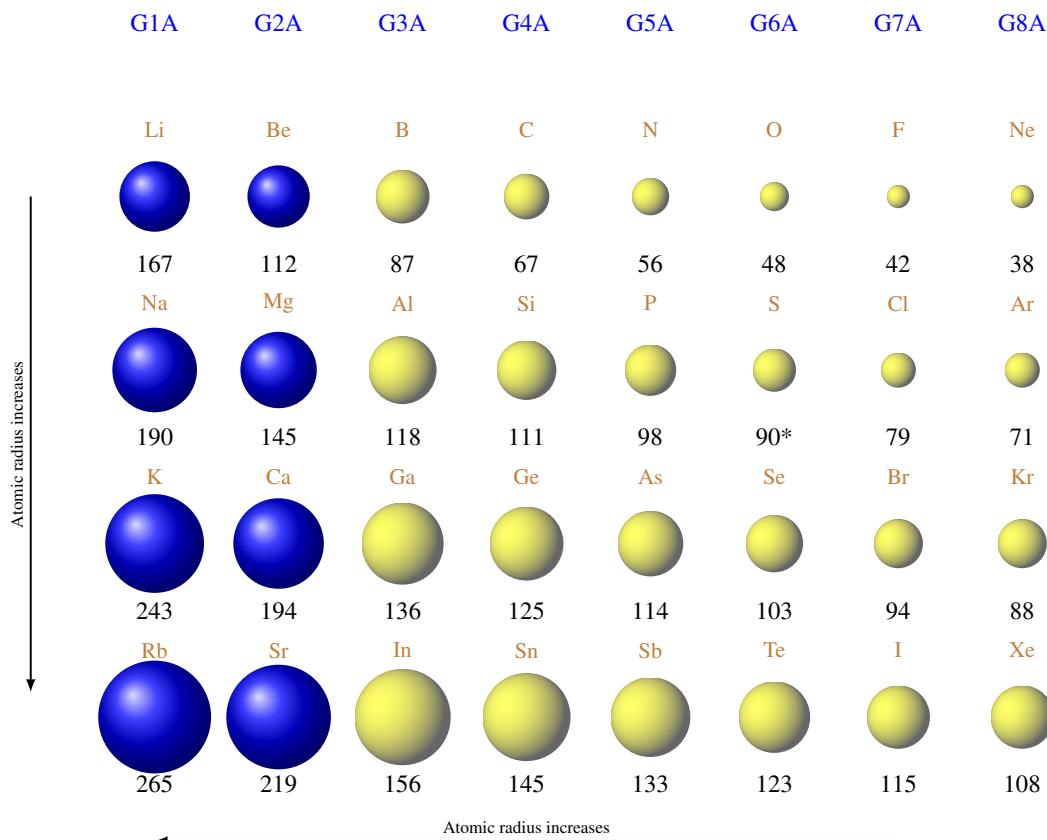


Figure 8.23 Change of atomic radius (calculated values given in pm) across the periodic table. The value with * was estimated

Table 8.6 Ionization energy in the periodic table in kJ/mol

Element	Z	EI ₁	EI ₂	EI ₃	EI ₄	EI ₅	EI ₆	EI ₇	EI ₈	EI ₉	EI ₁₀
Li	3	520.2	7298.1	11815.0							
Be	4	899.5	1757.1	14848.7	21006.6						*
B	5	800.6	2427.1	3659.7	25025.8	32826.7					
C	6	1086.5	2352.6	4620.5	6222.7	37831	47277.0				
N	7	1402.3	2856	4578.1	7475.0	9444.9	53266.6	64360			
O	8	1313.9	3388.3	5300.5	7469.2	10989.5	13326.5	71330	84078.0		
F	9	1681.0	3374.2	6050.4	8407.7	11022.7	15164.1	17868	92038.1	106434.3	
Ne	10	2080.7	3952.3	6122	9371	12177	15238	19999.0	23069.5	115379.5	131432

* Shaded cells represent the removal of core electrons

Atomic radii The size of atoms can not be specified exactly as the electron density of atoms stands throughout space. Still, we can arbitrarily define the atomic radii of atoms which are obtained by measuring distances between atoms in compounds. For covalent molecules, for example, O₂, we can measure the distance between the atoms in the molecule which is close to 150 pm, hence the atomic radius of oxygen—called the covalent atomic radius—should be close to 75pm. For metallic elements, we can



measure the metallic radii using the lattice spacing between atoms. In the periodic table, the atomic radii decrease from left to right of a period and increased from top to bottom of a group (see Figure 8.22 and 8.23)

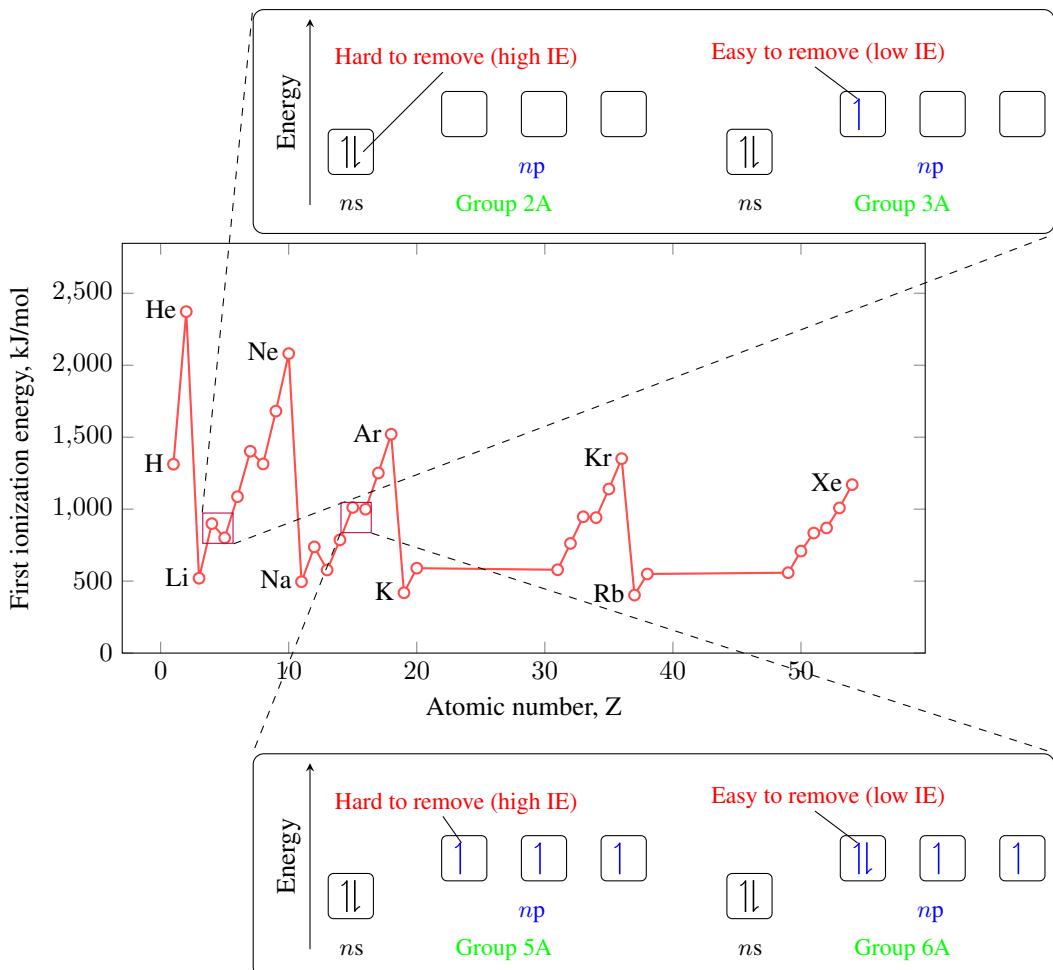
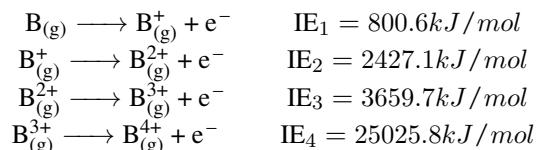
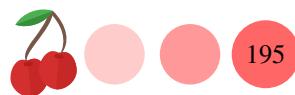


Figure 8.24 Ionization energy graphed with respect to the atomic number

Ionization Energy The *ionization energy* (IE) is the energy needed to remove an electron from an atom in a gas state and its fundamental (ground) electronic state. Atoms can have numerous ionization energies (see Table 8.6). The first ionization energy (IE_1) is the energy needed to remove the highest-energy electron on an atom, whereas the second ionization energy (IE_2) is the energy needed to remove the second highest-energy electron on the atom. For the case of boron,



Given the electron configuration of Boron ($[\text{He}]2s^22p^1$), the first electron comes from a p orbital, whereas the second comes from a s orbital, which lays closer to the nucleus. The fourth electron comes from the core and the fourth ionization energy is considerably higher than the rest. Overall, we have that ionizing an atom from p orbitals is less costly than ionizing from s orbitals, and ionizing an atom from core orbitals is more costly than ionizing from valence orbitals. The ionization energy increases (this means more energy is needed to remove an electron) going up a group and when going across



a period from left to right. In general, the ionization energy is low for metals and high for nonmetals. For example, if we compare the IE for H and He, as He is further right in the same period, it will have a larger IE and more energy will be needed to remove an electron ($IE_H < IE_{He}$). For the case of Li and H, the EI will be higher for H as it is further up in the same group ($IE_H > IE_{Li}$). There are discontinuities in the IE when moving across a period. Table ?? gives the IE for the second period. The first discontinuity happens between groups 2A and 3A as it is easier to remove p electrons than s electrons. The second discontinuity occurs between groups 5A and 6A as it is easier to remove an electron from a double occupied p orbital than from a single-occupied one.

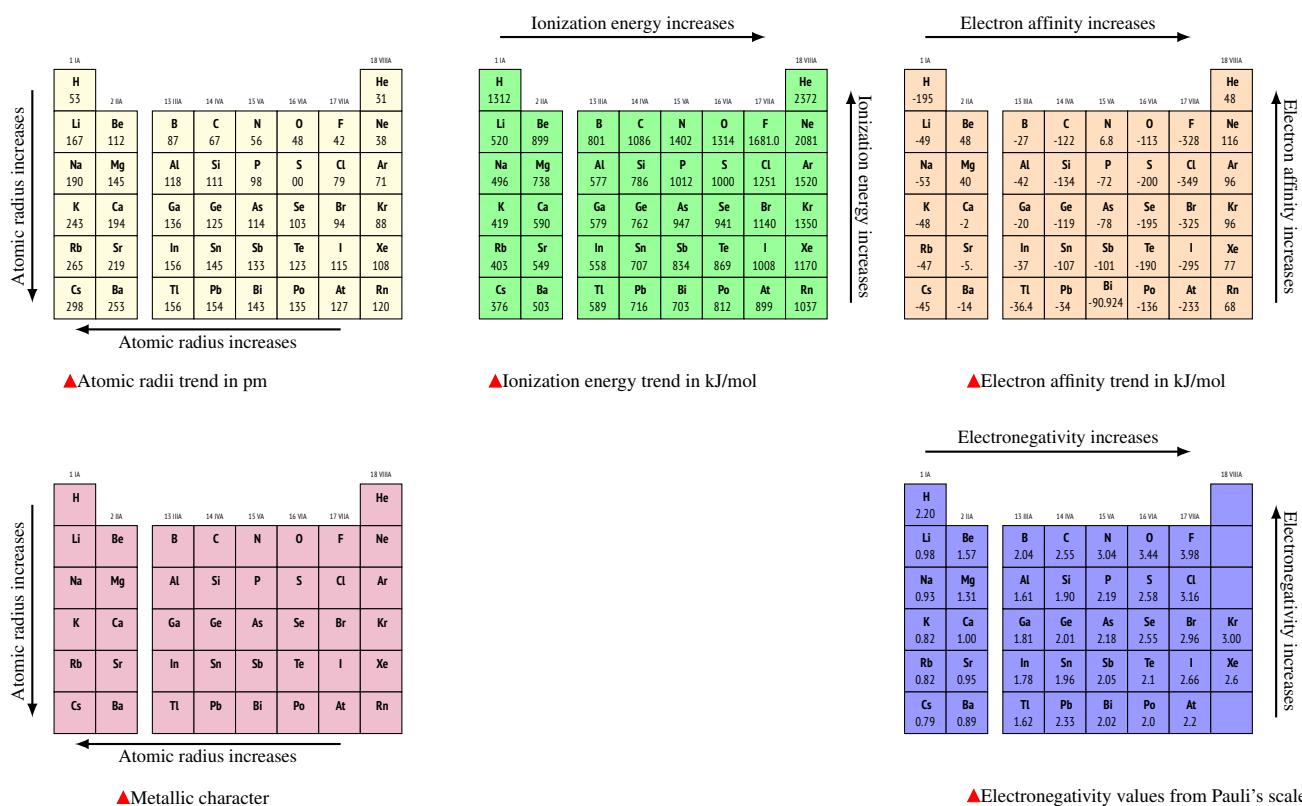


Figure 8.25 Periodic properties across the periodic table

Electron affinity The electron affinity (EA) represents the tendency of an atom to receive one or more electrons hence becoming negatively charged. Specifically, is the energy involved in the process of receiving an electron. As an example, the electron affinity of hydrogen is written as:



Here, we consider electron affinities as negative values so that the smaller (the more negative) this value the larger the tendency of the atom to accept electrons. In other words, it would be easier to add electrons to an atom with -10 kJ/mol EA, than to an atom with 10 kJ/mol EA. In the periodic table, EA decreases (becomes more negative) across a period from left to right. For example, EA for K is -48 kJ/mol and for Br is -325 kJ/mol . Hence, elements from the right of the table are more willing to gain electrons than elements from the left. On one hand, there are discontinuities in the electron affinity across a period. It is easier to add an electron to the elements in Group 1A than to elements in Group 2A, as an electron added to Group 2 elements would be



placed in *p* orbitals and these have higher-more positive-energies. Also, it is easier to add an electron to the elements in Group 4A than to elements in Group 5A, as an electron added to Group 4 elements would be placed in *p* orbitals giving three unpaired electrons, whereas electrons on Group 5 are all paired and a new electron would have to add to an already occupied orbital. On the other hand, there are fewer EA variations when going across a group. Finally, when adding more than one electron, the second EA tends to be more positive-less favored-than the first electron addition.

Electronegativity, EN Atoms combine by sharing or giving away electron density. The *electronegativity* of an atom in a molecule is its ability to attract electron density in a bond. Imagine two people holding a pillow with their hands, with the pillow representing a pair of electrons. If one of the people is more electronegative it will pull the pillow closer to them—it will attract more electrons. Electronegativity is loosely related to other periodic properties such as ionization energy and electron affinity. Very electronegative atoms such as F has also a large (negative) electron affinity (easily accepts electrons) and ionization energy (do not ionize easily). There are different electronegativity scales, and the most well-known scale was developed by Linus Pauling. Electronegativity (EN) increases (the atom is more electronegative) when going up a group (column) of the table and when going across a period (row), from left to right of the table. Highly electronegative atoms are located on the top right part of the table, whereas highly electropositive atoms are located on the bottom left part of the table. EN is a relative concept, that is, the electronegativity of an atom can only be measured about another atom. When comparing the EN of I and F, we found that F is more electronegative as it is further up in the same group ($EN_F > EN_I$).

Metallic character All elements in the periodic table have somehow a certain *metallic character* as they all can lose electrons as metals do—that is why metals are good conductors. The elements in the left part of the table are metals with a strong metallic character. Still, the elements on the right side of the table also have a certain metallic character (MC). The metallic character increases (the atom is more metallic) when going down a group (column) of the table and when going across a period (row) from right to left. For example, comparing K and Ca, we have that K is more metallic than Ca, as it is located further to the left in the same column ($MC_K > MC_{Ca}$). In the case of F and Cl, Cl is more metallic as it is located further down a group ($MC_{Cl} > MC_F$).

Sample Problem 95

Compare the following property for the given couple of elements: (a) Atomic radius of N and F. (b) Ionization energy of Na and Cs. (c) Electronegativity of F and I. (d) Metallic character of N and F.

SOLUTION

(a) You go from N to F by moving from left to right on a row of the periodic table, hence the radius of N is larger than the radius of F. This is because the atomic radius decreases from left to right on a row. (b) You go from Na to Cs by moving from up to down on a column of the periodic table, hence the ionization energy of Na is larger than for Cs. This is because the ionization energy decreases from top to bottom on a period. (c) You go from F to I by moving from down to up on a column of the periodic table, hence the electronegativity of F is larger than for I. This is because the electronegativity energy increased from bottom to top on a period. (d) You go from N to F by moving from left to right on a row of the periodic table, hence the metallic character of N is larger than for F. This is



because the metallic character increased from right to left on a period.

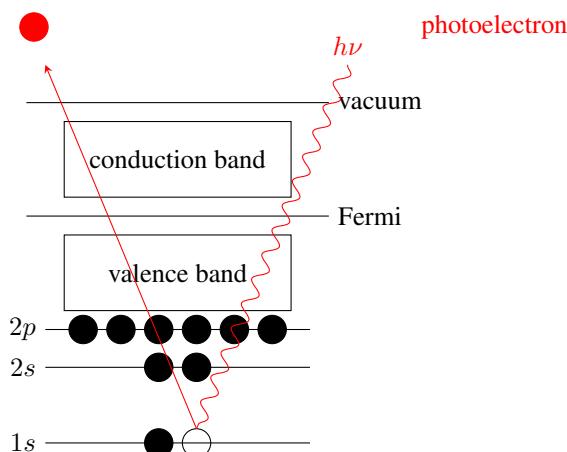
◆ STUDY CHECK

Compare the following property for the given couple of elements: (a) Atomic radius of F and I. (b) Electronegativity of Cs and Na.

Ionic radius Atoms gaining or losing electrons become ions. When an atom loses an electron it reduces its size. In particular, when an atom loses all valence electrons its size reduces considerably. When an atom gains an electron it gains size too as this new electron needs to be placed on an occupied orbital further away from the nucleus. Some ions have a common electronic configuration. For example, Na^+ and F^- both have the electron configuration: $[\text{He}]2\text{s}^22\text{p}^6$. Ions with the same electron configuration are called isoelectronic. For a series of isoelectronic ions, the larger the atomic number the smaller the ionic size due to the increase in nuclear attraction (see Figure ??).

8.13 Photoelectron spectroscopy of atoms

Figure 8.26 A photo-electron emitted from a 1s level



Photoelectron spectroscopy is a technique used to measure the relative binding of the electrons of an atom. It is useful to experimentally obtain the energy levels of an atom and properties such as the ionization energy. The principle behind the technique is similar to the photoelectric effect. By shining light with enough energy, one can remove electrons from an atom (see Figure 8.26). By measuring the kinetic energy of the ejected electron and taking into account the energy of the radiation we can estimate the binding energy of the ejected electron—called photoelectron—in the atom. The name, photoelectron spectroscopy, refers to the fact that electrons are ejected with light, by using photons. This technique is used to identify the presence of specific atoms as the photoelectron picks are element-specific, that is, each element presents a series of characteristic peaks. However, many factors affect the photoelectron picks and for example, a 1s peak of H can appear at different energies depending on the nature of the atom bonded to hydrogen. In general, on the vertical axis of a PES plot, you will find the relative intensity of the electrons and on the horizontal axis the energy of the photoelectron. The larger the energy the more strongly attached will be the electron in the atom and for example, a 1s peak will appear at higher energy than a 2s peak. The higher the intensity of the pick the larger the number of electrons in the level resulting in the photoelectron. For example, the intensity of a 1s^2 peak should be twice the intensity of a 1s peak. By comparing the intensity of the peaks



and the relative location one can identify the atom represented on the spectra (see Figure 8.27).

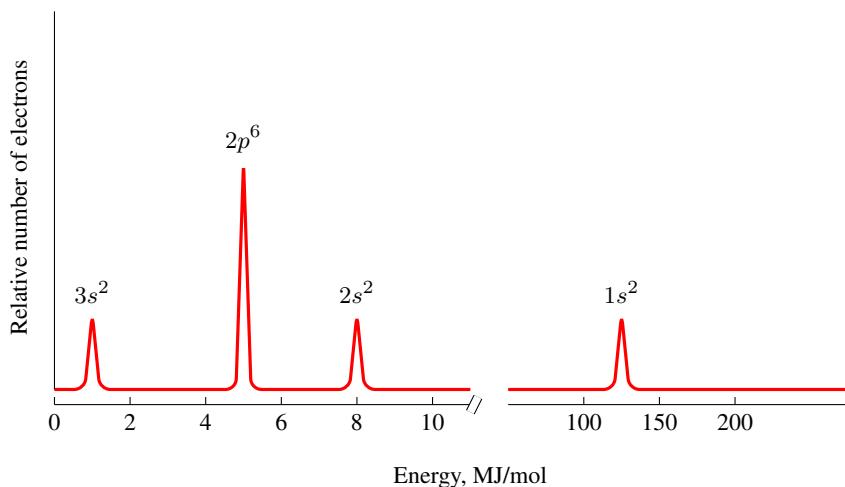


Figure 8.27 Photoelectron spectrum (PES) of Magnesium



CHAPTER 8

THE NATURE OF LIGHT

8.1 Calculate the following properties: (a) The energy in joules of a radiation with frequency 2.0×10^{18} Hz? (b) The frequency of a radiation with energy 5.6×10^{-20} J? (c) The energy in joules of a radiation with wavelength 653 nm?

8.2 Calculate the following properties: (a) The wavelength of a radiation with energy 5.34×10^{-16} J? (b) The wavelength of a radiation with frequency of 3.4×10^{14} Hz?

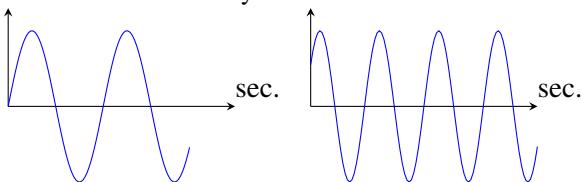
8.3 Calculate the following properties: (a) The color of a radiation with $\lambda = 590$ nm. (b) The color of a radiation with $\lambda = 600$ nm. (c) The color of a radiation with $\lambda = 530$ nm. (d) The color of a radiation with $\lambda = 580$ nm.

8.4 Calculate the following properties: (a) The color of a radiation with $\lambda = 470$ nm. (b) The color of a radiation with $\lambda = 490$ nm. (c) The color of a radiation with $\lambda = 580$ nm. (d) The color of a radiation with $\lambda = 510$ nm.

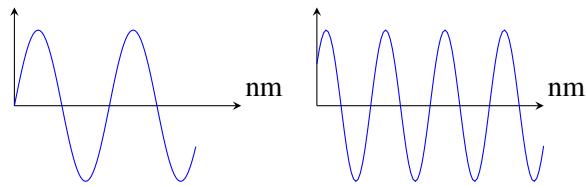
8.5 Classify the nature of a radiation (a) A radiation with $\gamma = 3.4 \times 10^8$ Hz (b) A radiation with $\gamma = 1.0 \times 10^{10}$ Hz (c) A radiation with $\gamma = 1.0 \times 10^{20}$ Hz (d) A radiation with $\gamma = 5.0 \times 10^{14}$ Hz

8.6 Classify the nature of a radiation (a) A radiation with $\gamma = 1.0 \times 10^{12}$ Hz (b) A radiation with $\gamma = 1.0 \times 10^5$ Hz (c) A radiation with $\gamma = 1.0 \times 10^{17}$ Hz (d) A radiation with $\gamma = 1.0 \times 10^{15}$ Hz

8.7 Sections of two electromagnetic waves A and B are represented below. Rank them in order of (a) increasing frequency; (b) increasing energy; (c) If wave B represents visible radiation, is wave A more likely to be IR or UV radiation?



8.8 Sections of two electromagnetic waves A and B are represented below. Rank them in order of (a) increasing wavelength; (b) increasing energy; (c) If wave B represents visible radiation, is wave A more likely to be IR or UV radiation?



THE ATOMIC SPECTRUM OF HYDROGEN

8.9 Which of these electron transitions correspond to absorption of energy and which to emission? (a) $\Delta E_{1 \rightarrow 2}$ (b) $\Delta E_{2 \rightarrow 1}$ (c) $\Delta E_{3 \rightarrow 1}$ (d) $\Delta E_{3 \rightarrow 5}$ (e) $\Delta E_{5 \rightarrow 3}$ (f) $\Delta E_{1 \rightarrow 3}$

8.10 Use the Bohr equation to: (a) find the energy of the photon emitted when an H atom undergoes a transition from $n = 1$ to $n = 4$. (b) find the wavelength (in nm) of the photon emitted when an H atom undergoes a transition from $n = 2$ to $n = 4$.

8.11 Use the Bohr equation to find the frequency (in Hz) of the photon emitted when an H atom undergoes a transition from $n = 1$ to $n = 5$.

8.12 An electron in the lowest energy level of H atom absorbs a photon of wavelength 96.97 nm. Indicate the final energy level of the electron moved.

QUANTUM MECHANICS

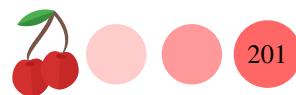
8.13 Indicate if the following combination of quantum numbers are allowed:

<i>n</i>	<i>l</i>	<i>m_l</i>	<i>m_s</i>	Allowed?
4	4	1	+1/2	
2	1	4	+1/2	
4	2	-2	-1/2	

8.14 Indicate if the following combination of quantum numbers are allowed:

<i>n</i>	<i>l</i>	<i>m_l</i>	<i>m_s</i>	Allowed?
0	1	2	+1/2	
1	0	0	+1/2	
2	1	1	-1/2	

8.15 For each of the following sublevels, give the values of the n and ℓ quantum numbers and indicate the number of orbitals in the sublevel: (a) 6s (b) 4d (c) 2p



8.16 For each of the following sublevels, give the values of the n and ℓ quantum numbers and indicate the number of orbitals in the sublevel: (a) 2p (b) 1s (c) 4f

8.17 Describe the shape of the following orbitals using the terms lobular, spherical, or lobular(dumbbell shape): (a) 3d (b) 1s (c) 2p (d) 2s

8.18 Describe the shape of the following orbitals using the terms lobular, spherical, or lobular(dumbbell shape): (a) 4p (b) 4d (c) 3p (d) 3s

8.19 Match the following statements with: (1) have the same shape (2) can fit the same number of electrons (3) belong to the same energy level (4) can fit the same number of electrons (a) 1s and 2s orbitals (b) five 3d orbitals (c) 2p and 3p sublevels (d) 3s and 3p sublevels

8.20 Match the following statements with: (1) have the same shape (2) can fit the same number of electrons (3) belong to the same energy level (4) can fit the same number of electrons (a) 4p and 3p orbitals (b) three 3p orbitals (c) 3d and 3s sublevels (d) 3p and 5p sublevels

8.21 Indicate the following: (a) orbitals in a 1s sublevel (b) sublevels in the fourth energy level (c) orbitals in the fourth energy level

8.22 Indicate the following: (a) orbitals in a 3p sublevel (b) sublevels in the third energy level (c) orbitals in the third energy level

8.23 Indicate the following: (a) the maximum number of electrons in a 3d sublevel (b) the maximum number of electrons in a 4f sublevel (c) the maximum number of electrons in a 1s sublevel

8.24 Indicate the following: (a) the maximum number of electrons in a 1s orbital (b) the maximum number of electrons in a 3d orbital (c) the maximum number of electrons in a 4f orbital

8.25 Indicate the number of orbitals that can have the following designations: (a) 2s (b) 3p (c) 0p (d) $n = 4$

8.26 Indicate the number of orbitals that can have the following designations: (a) 1d (b) $n = 1$ (c) 3d (d) 4f

8.27 What is the element with the electron configuration (a) $1s^2 2s^2 2p^6 3s^1$ (b) $[Ar]3d^5 4s^1$ (c) $1s^2 2s^2 2p^6 3s^1$ (d) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$

8.28 What is the element with the electron configuration (a) $1s^2 2s^2 2p^6 3s^2 3p^5$ (b) $1s^2 2s^2 2p^6 3s^2 3p^4$ (c) $[Kr]5s^2 4d^8$

8.29 Write down the abbreviated electron configuration for the following elements: (a) Cobalt (b) Chromium (c) Argon (d) Potassium (e) Chlorine (f) Vanadium

8.30 Write down the abbreviated electron configuration for the following elements: (a) Calcium (b) Manganese (c) Iron (d) Nickel (e) Copper (f) Titanium

8.31 Write down the full electron configuration for the following elements: (a) Barium (b) Samarium (c) Vanadium

8.32 Write down the full electron configuration for the following elements: (a) Aluminum (b) Potassium (c) Nickel

8.33 Write down the orbital diagram for the following elements: (a) Argon (b) Silicon (c) Sulfur (d) Chlorine

8.34 Write down the orbital diagram for the following elements: (a) Phosphorus (b) Boron (c) Carbon (d) Nitrogen

8.35 Indicate whether the following orbital diagram is possible for an atom on its fundamental state:



8.36 Indicate whether the following orbital diagram is possible for an atom on its fundamental state:



8.37 Indicate whether the following orbital diagram is possible for an atom on its fundamental state:



8.38 Indicate whether the following orbital diagram is possible for an atom on its fundamental state:





8.39 How many electrons are lost or gained by the following atoms when forming ions: (a) K (b) S (c) N (d) Ba (e) Ca (f) Mg

8.40 How many electrons are lost or gained by the following atoms when forming ions: (a) P (b) Li (c) Sr (d) Rb (e) Al (f) Cl

8.41 Write the ions formed by the following atoms:
(a) F (b) Cl (c) O (d) K (e) Cs (f) Sr (g) Al

8.42 Write the ions formed by the following atoms:
(a) Br (b) Li (c) Rb (d) Mg (e) Na (f) Ca (g) S

8.43 Write the ions formed by atoms with the following electron configuration: He 2s¹ He 2s² Ne 3s¹ Kr 5s¹

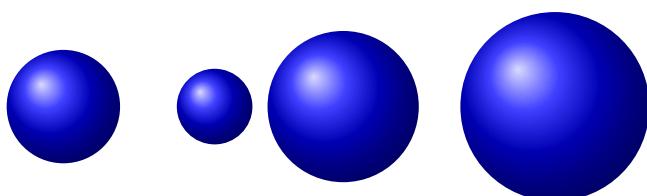
8.44 Write the ions formed by atoms with the following electron configuration: Xe 6s¹ Ne 3s²3p⁴ He 2s²2p⁴
(a) ns²

PERIODIC PROPERTIES

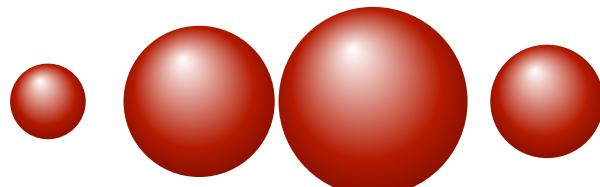
8.45 Among the elements, indicate the element with the largest atomic radius (a) B (b) C (c) F (d) Li (e) Na

8.46 Among the elements, indicate the element with the smallest atomic radius (a) C (b) N (c) O (d) S (e) Se

8.47 Match the spheres (far left, center left, center right, far right) with the atoms: Be, Li, Na, B



8.48 Match the spheres (far left, center left, center right, far right) with the atoms: P, S, Si ,Cl.



8.49 Among the elements, indicate the element with the largest electronegativity (a) B (b) C (c) F (d) Li

8.50 Among the elements, indicate the element with the largest electronegativity (a) Si (b) P (c) S (d) Se

8.51 Among the elements, indicate the element with the smallest ionization energy (a) B (b) C (c) F (d) Li (e) Na

8.52 Among the elements, indicate the element with the largest ionization energy (a) Al (b) Si (c) P (d) As (e) Sb

8.53 Among the elements, indicate the element with the largest metallic character (a) B (b) C (c) F (d) Li (e) Na

8.54 Among the elements, indicate the element with the largest metallic character (a) K (b) Rb (c) Cs (d) Ca

Ch. 9. Electronic structure of molecules

In nature molecules can be found in a myriad of different shapes. Some like carbon dioxide are one-dimensional or linear like methane have a shape that expands in the three directions of space—they have a three-dimensional shape. The shape of molecules results from the chemical bonds connecting atoms in a molecule and from the existence of lone pairs of electrons. This chapter covers the analysis of the molecular shape and gains insight into advanced models of the chemical bond. After studying the ideas in this chapter you will be able to draw the connections between the atoms of a molecule and draft Lewis structures used as graphical representations of the molecular bonds. At the end of the chapter, we will address the idea of molecular polarity, which results from the distribution of charge in a molecule. Polarity will understand the reasons why you use soap to get rid of oil while doing dishes.

9.1 Electron-dot structures of atoms & molecules

Protons, neutrons, and electrons make the atoms. Electrons—in particular valence electrons—are responsible for the main chemical properties of an atom. These electrons are loosely bound and can be exchanged easily with other atoms, in contrast to the strongly-tied core electrons. The electron-dot structure of an atom or a molecule—also called Lewis structures—is a visual representation of the electronic arrangement of the valence electrons. Atoms in a molecule will tend to be surrounded by eight electrons so that their electron configuration resembles a noble gas. This arrangement is known as the octet rule. This rule is responsible for the common negative charge of F, and the positive charge of Na: F ($[He]2s^22p^5$) can easily receive an extra electron producing ionic F^- ($[He]2s^22p^6 = [Ne]$), and atomic Na ($[Ne]3s^1$) can lose an electron producing ionic Na^+ ($[He]2s^22p^6 = [Ne]$). There are a few exceptions. A remarkable one is the case of the hydrogen atom that follows the duet rule.

Valence electrons of atoms, and molecules The electrons of an atom are divided into core electrons and valence electrons. The valence electrons of an atom are involved in chemical bonds as they are less bonded to the nucleus. *The number of valence electrons of an atom* corresponds to the group number. For example, hydrogen H belongs to the group IA, and hence it has one valence electron. Similarly, oxygen O belongs to the group VIA, having six valence electrons. Similarly, we can count the *number of valence electrons of a molecule* by adding the valence electrons of the atoms that make the molecule. For example, water (H_2O) has eight valence electrons as each oxygen has one valence electron and oxygen has six. The number of *pairs of electrons* is just the overall number of valence electrons divided by two. For example, water has



eight valence electrons that correspond to 4 pairs of electrons.

Sample Problem 96

Indicate the number of valence electrons for the following atoms: N, O, C and S, and the number of pairs of electrons of the following molecules: NH₃, and CO₂.

SOLUTION

Nitrogen is in group VA and hence it has five valence electrons ($5e^-$). Oxygen belongs to the group VIA and C belong to IVA, hence they have six and four valence electrons, respectively. For the molecules, we have that ammonia has 8 electrons (nitrogen has five valence electrons and each hydrogen has one electron) that correspond to four pairs, whereas carbon dioxide has 16 electrons (carbon has four electrons and each oxygen has six) and eight pairs.

◆ STUDY CHECK

Indicate the number of valence electrons for the following atoms: Cl and B.

The octet rule Atoms exchange electrons when they combine to form molecules. This electron exchange is the driving force that drives the formation of molecules from single atoms. The octet rule states that each atom in a stable molecule should be surrounded by eight (octet) electrons achieving noble gas electron configurations. There are two important exceptions to this rule as H is surrounded only by two electrons (this is called the duet rule), and B by six. This rule comes from the experimental observation of numerous molecules.

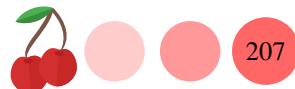
Electron-dot structure of an atom The electron-dot structure of an atom is a visual representation of the arrangement of the valence electrons of the atom. To write the electron-dot structure of an atom, you just need to write down the symbol of the atom surrounded by the valence electrons located in the four directions of the space: top, bottom, right, and left. To place the electrons, you start in any of the directions and fill one electron at a time. For example, for the case of three electrons, we would have: $\cdot\ddot{\text{B}}\cdot$. After all four directions have been filled, you need to start pairing the electrons. For example, for the case of five electrons, we would have: $\cdot\ddot{\text{P}}\cdot$. Another example, oxygen has six valence electrons and hence, the electron-dot structure would be $\cdot\ddot{\text{O}}\cdot$. Similarly, the electron-dot structure of fluorine would be $\cdot\ddot{\text{F}}\cdot$. For ions, you need to add (if its an anion) or subtract (if its a cation) valence electrons, and for example the electron-dot structure of the oxide anion O²⁻ is $:\ddot{\text{O}}:^{2-}$. The electron-dot structure of atoms is useful to predict—or make sense—of the atomic valence. Mind that the number of valence electrons of an atom is not the same as the valence of the atom. The valence of an atom is a number used to combine with other atoms forming compounds. For example, the electron-dot structure of nitrogen is $\cdot\ddot{\text{N}}\cdot$ and this atom needs to gain three electrons to reach the noble gas configuration with eight electrons $:\ddot{\text{N}}:^{3-}$ hence its valence is -3.

Sample Problem 97

Write down the electron-dot structure for the following atoms: N, C and Cl⁻.

SOLUTION

N has five valence electrons, whereas C has four. Hence the electron-dot for both will be: $\cdot\ddot{\text{N}}\cdot$ and $\cdot\ddot{\text{C}}\cdot$. Cl⁻ has eight valence electrons, that is seven plus

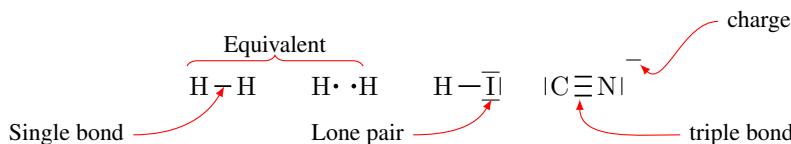


one, and hence its electron-dot structure will be $\text{Cl}^{\cdot\cdot-}$.

◆ STUDY CHECK

Write down the electron-dot structure for N^{3-}

An introduction to electron-dot structures Below, you will find some examples of electron-dot structures. Mind that the lines represent pairs of electrons hence below there are two equivalent representations for the hydrogen molecule. In these structures, you will find two different types of lines. Some pairs of electrons connect atoms. We call these types of pairs bonds. Other pairs lay on atoms. We call these lone pairs. Each atom can have a different number of lone pairs. For example, in the Lewis structures below carbon has one lone pair whereas iodide has three pairs. Bonds can be simple or multiple, double or triple. Finally, some molecules are charged and the charge is normally indicated on the top right side of the representation.



Electron-dot structure of diatomic molecules Electron-dot structures—or Lewis structures—of diatomic molecules are the most simple electron-dot structures of molecules that you will see. To obtain these structures, you need to follow the next steps. The first step is (1) to set up the atoms in the molecule in the form of a line. After that, (2) you need to count the total number of valence electrons in the molecule by adding the valence electrons of each atom (remember the number of valence electrons corresponds to the group number in the A notation). Then (3) compute the pairs of electrons represented by lines—the total number of valence electrons divided by two. Finally, (4) you need to start distributing the electron pairs in the molecule in a very specific way, first connecting the atoms among themselves, and then placing the remaining pairs surrounding the atoms. Following the octet rule, each atom except for H and B should be surrounded by four pairs, counting as pairs the bonds and lone pairs.

Sample Problem 98

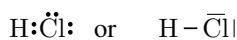
Construct the electron-dot structure of HCl.

SOLUTION

We first arrange the atoms in the molecule as indicated below and then we count the number of valence electrons: H(1) and Cl(7) that gives a total of eight electrons. We have four pairs of electrons.



Now we distribute the pair on each atoms knowing that each atom has to have four pairs with the exception of hydrogen that can only be surrounded by one pair. We can use lines instead of pairs



◆ STUDY CHECK

Construct the electron-dot structure of HF.



Number of bonds and atomic nature The number of covalent bonds that a nonmetal form is related to the number of electrons needed to complete the octet. For example, Hydrogen ($1s^2$) tends to form one bond to make compounds, whereas Nitrogen ($[He]2s^22p^3$) forms three bonds. For example, in the NH_3 molecule, each H forms one bond whereas N forms three bonds. Table 9.1 gives the relation between the number of bonds formed by several elements.

Table 9.1 Relation between the number of bonds and the atomic nature

1A	3A	4A	5A	6A	7A
H					
1 bond					
	B	C	N	O	F
	3 bonds	4 bonds	3 bonds	2 bonds	1 bonds
		Si	P	S	Cl, Br, I
		4 bonds	3 bonds	2 bonds	1 bond

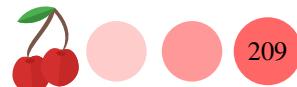
Electron-dot structure of general molecules Now we will address how to build up electron-dot structures of more complex molecules given that one of the atoms is the central atom and the others are connected to this central atom. The first step is (1) to arrange the atoms in the molecule, in the form of a central atom and the remaining atoms around it; the central atom is the one with a lower index in the molecule (e.g. in H_2O is O or in NH_3 is N). After that, (2) you need to count the total number of valence electrons in the molecule, dividing this number by two to obtain the number of pairs of electrons represented by lines. In the following (3) you need to connect the surrounding atoms to the central atom with electron pairs, and then (4) place electron pairs on top of the surrounding atoms, always placing a maximum of four atoms. Finally (5) place the remaining pairs in the central atom. Overall, each atom should be surrounded by four pairs (this is the octet rule) except H and B which should be surrounded by one and three pairs respectively. When drawing Lewis structures it is not important the atom arrangement (if the molecule looks like a line, a triangle or so) as long as the connectivity (which atom goes in the center and the surroundings) is correct.

Sample Problem 99

Construct the electron-dot structure of H_2O indicating the number of bonds and lone pairs.

SOLUTION

- 1 **Step one:** we first arrange the atoms in the molecule as H O H. The central atom is O as oxygen has the lower index in the H_2O molecule—the index for O is one and the index for H is two.
- 2 **Step two:** now we count the total number of valence electrons, including all atoms: $2 \times \text{H}(1)$ and $\text{O}(6)$ that gives a total of eight electrons.
- 3 **Step three:** let us count the pairs of electrons; we have eight electrons and that is four pairs.
- 4 **Step four:** now we distribute the pair on each atoms knowing that each

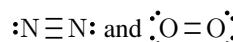


atom has to have four pairs with the exception of hydrogen that can only be surrounded by one pair. $\text{H}:\ddot{\text{O}}:\text{H}$: and using lines instead of pairs (this is not necessary but makes the electron-dot structure look better) we obtain $\text{H}-\overline{\text{O}}-\text{H}$. The molecule has two bonds, each one connecting an H to the oxygen atom and two lone pairs located on the oxygen atom.

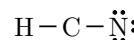
STUDY CHECK

Construct the electron-dot structure of NH_3 indicating the number of bonds and lone pairs.

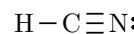
Multiple bonds Often you are going to encounter electron-dot structures like the ones below



in which the atoms are connected through multiple bonds, double or triple bonds. Multiple bonds are formed while constructing electron-dot structures to impose the octet rule. Look for example the lewis structure for the HCN molecule below



In this structure, carbon does not follow the octet rule. We can enforce the octet rule by moving lone pairs from the atoms into the bond forming the structure below



In this structure both carbon and nitrogen follow the octet rule. Hence, we need to add one more step to the Lewis structure construction scheme: convert lone pairs of electrons into bonds to enforce the octet rule.

Sample Problem 100

Construct the electron-dot structure of O_2 .

SOLUTION

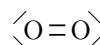
- Step one:** We first arrange the atoms in the molecule as



Now we count the total number of valence electrons, including all atoms: $2 \times \text{O}(6)$ that gives a total of twelve electrons. Let us count the pairs of electrons; we have twelve electrons and that is six pairs. Then we distribute the pairs, first connecting the atoms $\text{O} - \text{O}$ (we have five extra pairs to distribute at this point), and we place the remaining pairs on top of the oxygen atoms



The right oxygen do not follow the octet rule. In order to enforce the octet rule we move lone pairs into the bond



STUDY CHECK

Construct the electron-dot structure of CO_2 .



Atomic charges in a molecule The electron-dot structure of a molecule results from counting the overall number of valence electrons of the molecule given that each atom brings a different number of valence electrons (n_e^{free}). For example, two H atoms bring one electron each, whereas O brings two electrons, giving a total of six valence electrons. When arranging the electron pairs in the molecule, the number of electrons surrounding an atom is called the valence of this atom in the molecule (n_e^{bonded}). We calculate the number of valence electrons of an atom in a molecule by accounting for the number of lone pairs on this atom and half the number of bonds:

$$n_e^{bonded} = \text{number of lone pairs} + 1/2\text{number of bonds}$$

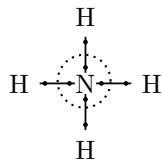
It is important to note that the valence of a free atom and the valence of this atom in a molecule is not necessarily the same. Indeed the difference between the valence electron of a free atom and the same atom in a molecule is the effective charge of that atom in the molecule, Q :

$$Q_{eff} = n_e^{free} - n_e^{bonded}$$

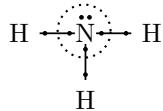
When the valence of an atom in a molecule is larger than the valence of the free atoms we have negative effective charges. In the example below



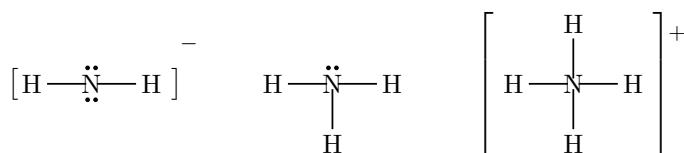
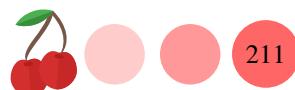
the number of electrons surrounding nitrogen is six electrons, more than the number of electrons originally brought to the molecule (five). We conclude that the atoms have a negative charge, and the effective atomic charge of nitrogen is $Q=-1$. In the next example,



the central atom, nitrogen, still has five valence electrons. After counting the electrons surrounding nitrogen, this time we find that this atom is surrounded by four electrons, less than the number of electrons originally brought to the molecule. We can conclude that nitrogen has a positive charge. In particular, the effective atomic charge of nitrogen in this molecule is the number of valence electrons minus the number of surrounding electrons. In this case, the atomic charge is $Q=+1$. When the valence of an atom in a molecule is the same as the valence of the free atoms we have zero effective charges. In this last example



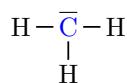
the central atom, nitrogen, has five valence electrons. After counting the electrons surrounding nitrogen—remember in a bond each atom shared an electron and hence each line around an atom counts as one electron—we find that this atom is surrounded by five electrons. As the number of valence electrons brought to the molecule is the same as the number of electrons surrounding the atom, we say the atomic charge of this atom is zero ($Q=0$). Hence, the atom is neutral. In all the molecules above, hydrogen remains neutral and hence the atomic charge of nitrogen corresponds to the molecular charge of the molecule. We can hence summarize the three scenarios indicated, as we have a neutral molecule in the center, a positive molecule on the right, and a negative molecule on the left.



The atomic charge of an isolated atom can be well-defined. However, the atomic charge of an atom in a molecule is arbitrarily defined, and more than one definition exists. Formal charges are one of the possible definitions of atomic charges in a molecule, whereas redox numbers are an alternative definition of atomic charges in molecules. None of these definitions is exactly correct. For example, redox numbers tend to overestimate the atomic charges, as they assume that all shared electrons in a bond belong to the most electronegative atom. Normally, negative formal charges tend to reside on electronegative atoms and not on electropositive atoms. At the same time, the sum of all effective charges needs to give the overall charge of the species. Furthermore, atoms in molecules tend to achieve formal charges as close to zero as possible. One can use formal charges to assess the validity of a Lewis structure. When comparing a series of equivalent Lewis structures for a molecule, the structures that best describe the bonding in the molecule tend to be those with small effective charges located on electronegative atoms.

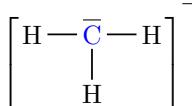
Sample Problem 101

Indicate the atomic charges of the blue highlighted atom



SOLUTION

The carbon atom brings four electrons and in the molecule it is surrounded by eight electrons, five of which belongs to it. Hence the charge of C is -1 ; this means that carbon has one extra electron. Each hydrogen brings one electron and in the molecule each hydrogen has one electron (they share two electrons with C, one for C and one for H). The final lewis structure with the local charge of carbon can be indicated as:



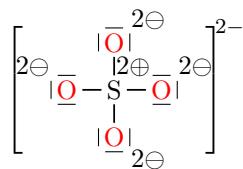
◆ STUDY CHECK

Indicate the atomic charges of all atoms in the Lewis structure below

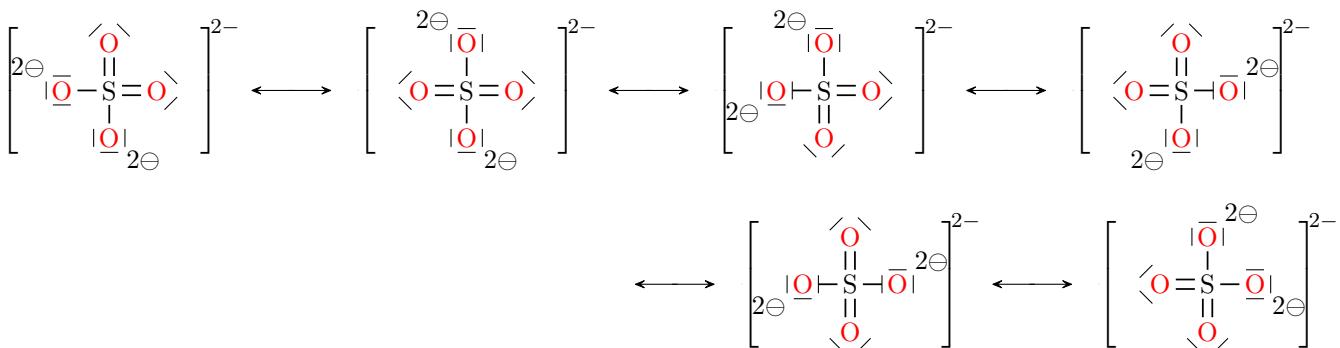


Resonant structures Let us analyze the Lewis structure of the sulfate ion, SO_4^{-2} .

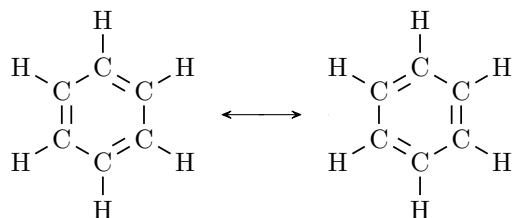
The goal is to analyze the Lewis structure to gain insight into the bonding state of the molecule, with an emphasis on the S–O bond length. The total number of electrons in the ion is 32, which corresponds to 16 pairs. We will first set up the atomic structure of the ion, using sulfur as a central atom, and connect the central atom to the surrounding oxygens using four pairs of electrons. Still, we have pairs of electrons that will be localized as lone pairs on the oxygen atoms given the structure below:



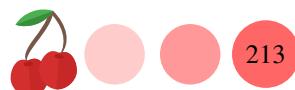
The structure above is a valid Lewis structure. However, it does not accurately represent the bonding of the sulfate ion, as the formal charges are very high: the formal charge of S is +2 and the formal charge of each O is -1, giving the overall ionic charge of -2. All oxygen atoms and sulfur follow the octet rule. Still, the charge on sulfur can be minimized by moving two lone pairs into a bond. There are several ways to do this movement. Indeed there is no reason to choose a particular oxygen atom to generate a double bond. In particular, one can think of six equivalent but yet different Lewis structures listed below:



Often there are several equivalent lewis structures for the same molecule. These structures do not differ in the atomic connections but in the electron distribution. For these situations, we say there is resonance between the different structures. Resonance exists on the sulfate ion, hence the bonds are neither single nor double, all S-O bonds are equivalent, with equivalent lengths. The arrows above indicate that all structures are equivalent, and it does not represent any type of equilibrium. The concept of resonance is in contrast with the assumption of the Lewis structures which are based on a localized bond model: molecules contain localized bonds and lone pairs. However, this model is less than perfect and goes against the quantum nature of the electron in which electrons exist in a delocalized state. The existence of resonance has other strong consequences. Molecules with numerous resonant structures are stabilized by resonance. This means they are more stable than equivalent molecules without resonance. For example, benzene—a molecule with 15 pairs of electrons—is a very stable molecule with two resonant structures which stabilize its structure.



Exceptions to the octet rule The octet rule assumes that all atoms are surrounded by eight pairs of electrons (either lone pairs or bonds) as atoms tend to achieve a stable noble gas configuration. However, not all atoms follow the octet rule. It is fair to say that most of the second-period atoms, C, N, O, and F follow the octet rule. Hydrogen does not follow the octet rule. It follows the duet rule of being surrounded by a single pair of electrons. Similarly, Boron does not follow the octet rule and tends to



form a maximum of three bonds. The Lewis structure of a boron compound is presented below:



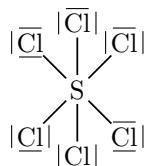
Boron and hydrogen have a reduced octet, with less than eight electrons. At the same time, atoms belonging to the third period (e.g. S, P) do not tend to follow the octet rule. They tend to have an expanded octet, surrounded by more than eight electrons. This is because the model behind the octet rule, the localized electron model, assumes that all atoms use their s and p orbitals to create bonds. However, atoms in the third period can also use the d orbitals which can fit extra pairs of electrons. The Lewis structure of a phosphorous compound is presented above. When dealing with expanded octets it is safe to assume that the central atom locates the expanded octet and hence the extra pairs of electrons.

Sample Problem 102

Obtain the Lewis structure of SCl_6 .

SOLUTION

We have that in the sulfur hexachloride molecule, sulfur is connected to six chlorine atoms. Hence, in this molecule, sulfur has an expanded octet. Let us first count the number of electrons and pairs of electrons. The valence of sulfur is six and the valence of chlorine is seven. Overall we have 48 electrons and 24 pairs. The Lewis structure of this molecule will be:



❖ STUDY CHECK

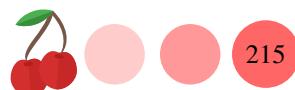
Obtain the Lewis structure of I_3^-

Molecules with odd number of electrons Lewis structures are based on localized electron models that assume that molecules are made of atoms connected through pairs of electrons. Some molecules have an odd number of molecules and for those, the localized electron model does not work. An example is nitrogen monoxide NO which has eleven electrons. Nitrogen monoxide forms as a result of the combustion of gasoline in car engines. The localized electron model does not handle well molecules with an odd number of electrons and more advanced models would be required to describe the bonding state of these molecules.



Table ?? Molecular geometries

Electron groups (AEs)	Electron-group geometry	Bonded atoms (Bs)	Lone pairs (Es)	ABE Code	Molecular shape	Bond Angle	3D model
2	Linear	2	0	AB ₂	Linear	180°	
3	Trigonal Planar	3	0	AB ₃	Trigonal Planar	120°	
3	Trigonal Planar	2	1	AB ₂ E	Bent	120°	
4	Tetrahedral	4	0	AB ₄	Tetrahedral	109°	
4	Tetrahedral	3	1	AB ₃ E	Trigonal pyramidal	109°	
4	Tetrahedral	2	2	AB ₂ E ₂	Bent	109°	
5	trigonal bipyramidal	5	0	AB ₅	trigonal bipyramidal	90°, 120°, 180°	
6	octahedral	6	0	AB ₆	octahedral	90°, 180°, 180°	
5	trigonal bipyramidal	4	1	AB ₄ E	see-saw	180°, 120°, 90°	
5	trigonal bipyramidal	3	2	AB ₃ E ₂	T-shaped	90°, 180°	
5	trigonal bipyramidal	2	3	AB ₂ E ₃	Linear	180°	
6	octahedral	5	1	AB ₅ E	square pyramidal	90°	
6	octahedral	4	2	AB ₄ E ₂	square planar	90°, 180°	



Steps to obtain Lewis structures The following steps can be used to obtain the Lewis structure of a general molecule:

- 1 **Step one:** Arrange the atoms in the molecule, in the form of a central atom and the surrounding atoms
- 2 **Step two:** Obtain the number of pairs of valence electrons by dividing the total number of valence electrons of the molecule by two
- 3 **Step three:** Connect the surrounding atoms to the central atom with electron pairs
- 4 **Step four:** Place electron pairs on top of the surrounding atoms, always placing a maximum of four atoms
- 5 **Step five:** Place the remaining pairs in the central atom.
- 6 **Step six:** Convert lone pairs of electrons into bonds to enforce the octet rule
- 7 **Step seven:** For extended octets place the extra electrons on the central atom
- 8 **Step eight:** When numerous equivalent Lewis structures exist, the best structures would have low formal charges, with negative charges located on electronegative atoms

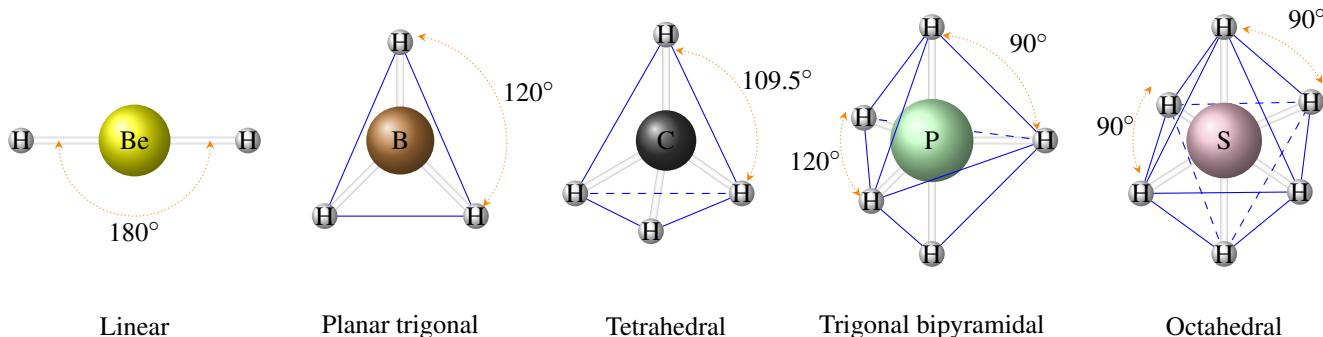
9.2 Molecular shape

Molecules consist of arrangements of atoms presented in different forms. Let us use as an example the H₂O molecule, which contains two hydrogen atoms and one oxygen. Knowing that both hydrogens are connected to oxygen through a covalent bond, one can envision several molecular geometries such as a linear geometry or maybe a v-shaped geometry with oxygen at the point. The geometry of a molecule determines its properties, and small geometrical changes can have severe consequences on the functioning of molecules. For example, at high temperatures, when proteins in the body denaturalize losing their unique structure they also lose their functionality. The goal of this section is to identify the approximate shape of a given molecule.

The VSEP model The VSEPR model, also known as the valence shell electron-pair repulsion model, is a model that predicts the geometries of molecules made of nonmetals. This model predicts the atomic arrangement of the molecules with an emphasis on the shape of the arrangement. However, it is not a very accurate model to predict geometries and there are better methods to obtain molecular geometries. The model predicts, for example, that water molecules have a v-shaped geometry and not a linear geometry while giving an estimate of the angle between the two O-H bonds. Still, VSEPR is not accurate enough to predict the O-H bond length and more advanced methods should be used for this purpose. The VSEPR model is based on the premise that the structure around a given atom results from minimizing the electron-pair repulsion. This way, the bonding and nonbonding pairs of electrons around a central atom are differently accounted for. Let us analyze a few cases in which the central atom only has bonding pairs of electrons. For example, the BeH₂ molecule has two bonding pairs around Be and the arrangement that maximizes the distance between both pairs hence minimizing repulsion is a linear arrangement. Hence, the BeH₂ molecule is linear with a 180° angle between both Be-H bonds. Another example would be the BH₃ molecules, a molecule with three bonding pairs. The geometry that maximizes the distance between

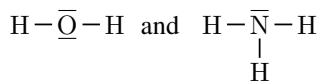


the three pairs hence minimizing repulsion is a trigonal planar structure in which the three bonding pairs are in the same plane with an angle of 120° between the three bonds. A final example would be the methane molecule (CH_4), a molecule with four bonding pairs. A tetrahedral arrangement with 109.5° between the C-H bonds is the most stable arrangement for this case.



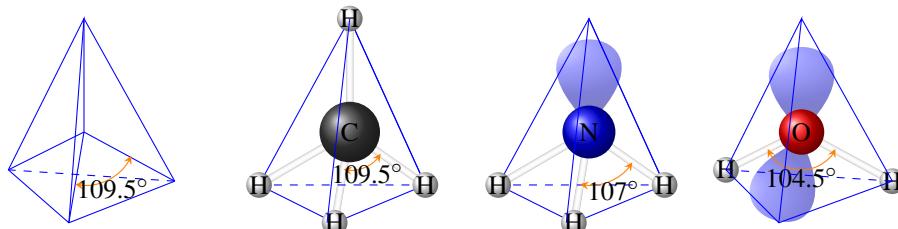
For the case of five bonds, the geometrical arrangement that minimizes the electron-pair interaction is a trigonal bipyramidal arrangement consisting of two pyramidal arrangements sharing a common base. The PH_5 molecule presents this arrangement. In this arrangement, there are two different bond angles: 90° between the vertical and in-plane and 120° for the in-plane bonds. Finally, the octahedral structure minimizes the pair repulsion in the case of six bonds and for example, the SH_6 molecule has an octahedral arrangement. In this arrangement, all bonds have a 90° angle. All atomic arrangements discussed above are presented in the diagram below.

ABE Molecular code We will use the ABE code to identify the molecular geometry of more complex molecules, with bonds and lone pairs. This code is based on the Lewis structure of the molecule, with B refers to the number of atoms connected to the central atom in the molecule (number of bonded atoms), and E is the number of lone pairs on the central atom. The overall number of bonded atoms and lone pairs is called the number of electron groups. Corresponding geometry for different ABE codes is tabulated. For example, an AB_2 molecule will be linear, whereas an AB_2E_2 is bent. The electron-dot structure of water and ammonia are:



Water has two bonds with the central atom and hence two Bs and two lone pairs on top of the central atom and hence two Es. The ABE code of water is AB_2E_2 and its geometry is bent. The ABE code of ammonia is AB_3E , as the molecule has three atoms connected to the central nitrogen and N has a single lone pair. Its geometry would be trigonal pyramidal. Angles between the different bonds for the different atomic arrangements are also tabulated. For example, the angle between the two H-O bonds of water would be 104.5° , whereas the angle between two of the N-H bonds of ammonia would be 107° . The overall number of bonding and lone pairs is referred to as the number of electron regions and the molecular geometry of the molecule is not necessarily the geometry of the electron regions. For example, the molecule methane has four bonds and a tetrahedral geometry. Ammonia has two bonds and two lone pairs. The geometry of the electron regions is also tetrahedral with three bonds pointing toward the lower part of the tetrahedron and the lone pair pointing toward the upper part. At the same time, the molecular geometry of ammonia is trigonal pyramidal. For the case of water,

we have that again the geometry of the four electron regions is tetrahedral whereas the molecular geometry is bent. We can also conclude that lone pairs require more room than bonding pairs and this has an impact on the molecular angles. For example, the angle between two bonds in a tetrahedron is 109.5° being this value is the same as the molecule angles of methane. Differently, the molecular angles of ammonia—a molecule with one lone pair—are 107° , and the molecular angle of water—a molecule with two lone pairs—is 104.5° . These results indicate that as the number of lone pairs increases the bonding pairs are more squeezed together.



Sample Problem 103

Identify the geometry of the following molecules: BF_3 and SO_2 .

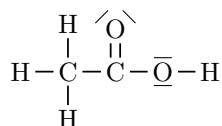
SOLUTION

We need first the electron-dot structure of both molecules. For BF_3 $|\overline{\text{F}}|-\text{B}-\overline{\text{F}}|$. The code of this molecule is AB_3 and hence its geometry would be trigonal planar. The correct way to draw the molecule respecting its geometry would be: $|\overline{\text{F}}|\text{B}-\overline{\text{F}}|$. The electron-dot structure for sulfur dioxide—remember this is covälfen molecule—is $|\underline{\text{O}}=\overline{\text{S}}=\underline{\text{O}}|$ and its class is AB_2E . Hence the molecular geometry is linear.

❖ STUDY CHECK

Identify and draw the geometry of methane (CH_4).

Complex molecules and multiple bonds To identify the ABE code we need to identify first the central and peripheral atoms. For some more complex molecules, there might not seem to be a central atom. An example of this case can be found in acetic acid.



In the molecule we have a carbon atom connected to three hydrogens and to another carbon which at the same time is connected to two oxygens, one of these is also connected to the final hydrogen. For this case, we just need to identify different geometry centers, that is, atoms that are central to the other connections and which are connected to at least two atoms. For this molecule, we have three central atoms. For each central atom, there will be a molecular arrangement. For example, the ABE code for the left carbon is AB_4 whereas for the right carbon is AB_3 . The geometry for the left-center would be tetrahedral, whereas for the right center would be planar



trigonal. The right oxygen is also a central atom connected to carbon and hydrogen. The ABE code for this center is AB₂E₂ and the geometry is bent. Furthermore, in the ABE code double bonds count as a single bonding pair. For example, the Lewis structure of carbon dioxide is: $\text{O}=\text{C}=\text{O}$. The ABE code for carbon dioxide would be AB₂ and its geometry would be linear with a 180° angle between the two C=O bonds. In the case of resonance, with several Lewis structures contributing to the chemical bond, any structure would predict the VSEPR geometry. Finally, it is important to stress that the VSEPR model is just a simple model and we should be careful when predicting quantitative information. For example, we have that both molecules ammonia and phosphine, NH₃ and PH₃, both with code AB₃E have a trigonal pyramidal geometry. However, whereas the experimental bond angle of ammonia is 107°—close to the value predicted by the model—the bond angle for phosphine is 94°—very different than the angle predicted by the VSEPR model. Still, this model is good enough to predict general molecular structures.

Steps to use the VSEPR model The following steps can be used to obtain the molecular geometry using the VSEPR model:

- 1 **Step one:** Identify the central and the peripheral atoms.
- 2 **Step two:** Obtain the Lewis structure of the molecule
- 3 **Step three:** Obtain the ABE code with B being the number of peripheral atoms and E being the number of lone pairs. A represents the central atom. Multiple bonds (double, triple) count as a single B.
- 4 **Step four:** Use Table ?? to obtain the molecular geometry

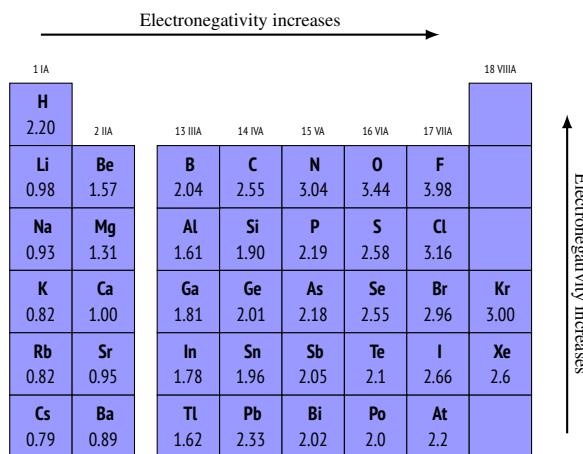


Figure 9.3 Electronegativity across the periodic table

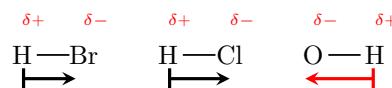
9.3 Polarity of molecules

This section deals with bond and molecule polarity. A chemical bond will be polar or nonpolar depending on the tendency of the atoms in a bond to attract the electrons in the bond. Polar bonds result in the existence of a permanent dipole moment that makes a molecule polar. Polar molecules can interact with polar molecules and mix.

Bond polarity Differences in electronegativity (see Figure 9.3) can be used to classify a chemical bond as covalent or ionic (see Table 9.4). On one hand, when the



electronegativity difference (ΔEN) of the atoms in the bond is less than 0.4 we will say the bond is *nonpolar covalent*. Examples are the H–H ($\Delta EN=0$) or C–H ($\Delta EN=0.2$) bonds. In these cases, the electrons are shared equally in the bond leading to a lack of charge distribution. On the other hand, a bond is *polar covalent* when the atoms bonded are different or have an electronegativity difference between 0.4 and 1.8. Examples are H–Br ($\Delta EN=0.8$), H–Cl ($\Delta EN=1.0$), or O–H ($\Delta EN=1.2$). Bonds become more polar as the electronegative difference in the bond increases. In polar covalent bonds, each atom shares the electrons in the bond unevenly which creates a *dipole moment*, a permanent charge separation. In the examples above, bromine or chlorine is more electronegative than hydrogen being more prone to attract the electrons than H. Br and Cl are partially negative Cl $^{\delta-}$ because of the negatively charged electrons and H is partially positive H $^{\delta+}$ because of the lack of electrons. We represent the excess of charge as on Cl or Br as Cl $^{\delta-}$ and electron deficiency in H as H $^{\delta+}$. The polarity of the bond is represented with an arrow pointing from the less electronegative, from positive, to the more electronegative atom so that the larger the electronegative difference the larger the dipole moment:



Finally, a bond is *ionic* when the atoms bonded have an electronegativity difference larger than 1.8. Examples are Na–Cl ($\Delta EN=2.2$), K–Cl ($\Delta EN=2.3$), or K–Br ($\Delta EN=2.1$). For such a large electronegativity difference, electrons are transferred from one atom to the other creating positive and negative ions in the bond. Ionic bonds are also polar due to the permanent charge distribution between the ions forming the bond. Mind that the variations in the type of bond are continuous and there is no defined point at which a bond stops being covalent to become ionic.

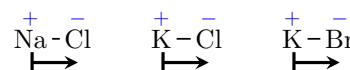


Table 9.4 Electronegative (EN) differences and types of bond

Electronegative Difference	0	0.4	1.8
Bond type	Nonpolar covalent	Polar covalent	Ionic
Electron Sharing	evenly	unevenly	electron transfer
	C–H	O–H	Na $^{+}$ –Cl $^{-}$

Polarity of molecules: *diatomic molecules* Molecules can either be polar or nonpolar. Polar molecules have a permanent dipole moment resulting from one or more polar bonds. Nonpolar molecules have no permanent dipole moment resulting either from nonpolar bonds or from a combination of polar bonds that lead to no dipole moment. The polarity of diatomic molecules, small molecules with only two atoms, only depends on the nature of the atoms that form the molecule. If the atoms in the molecule are the same (e.g. H₂ or O₂) or have similar electronegativities, then the molecule would be nonpolar. If the atoms are different with electronegativity difference between

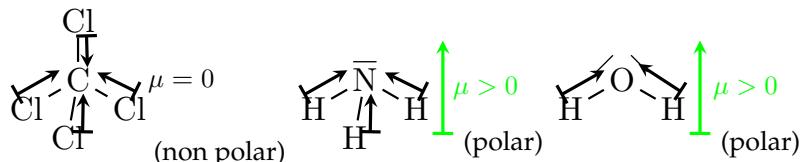


0.4 and 1.8 then the molecule would be polar. Examples are H₂ a nonpolar molecule whereas HCl or HBr are both polar molecules. See Table 9.5 for more examples.

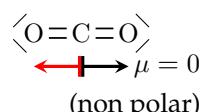
Table 9.5 Bond polarity differences in terms of electronegative (EN) differences

Bond	Electron Sharing	EN Difference	Type of bond
H—H	Evenly	0.0	Nonpolar covalent
C—H	Evenly	0.2	Nonpolar covalent
$\begin{array}{c} \delta+ \\ \\ H-Br \\ \\ \delta- \end{array}$	Unevenly	0.8	Polar covalent
$\begin{array}{c} \delta+ \\ \\ H-Cl \\ \\ \delta- \end{array}$	Unevenly	1.0	Polar covalent
$\begin{array}{c} \delta+ \\ \\ H-O \\ \\ \delta- \end{array}$	Unevenly	1.2	Polar covalent
$\begin{array}{c} + \\ \\ K-Br \\ \\ - \end{array}$	Electron transfer	2.1	Ionic
$\begin{array}{c} + \\ \\ Na-Cl \\ \\ - \end{array}$	Electron transfer	2.2	Ionic
$\begin{array}{c} + \\ \\ K-Cl \\ \\ - \end{array}$	Electron transfer	2.3	Ionic

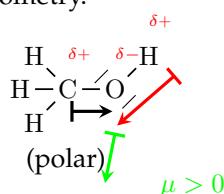
Polarity of larger molecules The polarity of larger molecules depends on the molecular geometry as well as the polar nature of the bonds that form the molecule. Let us analyze a few cases, H₂O, NH₃ and CCl₄. On one hand, for the H₂O case, the H—O bond is polar. The ABE type of water of AB₂E₂ and hence its geometry is bent; both H—O bonds do not compensate as they point in different directions and the directions do not cancel out what makes the water molecule polar having a permanent dipole moment ($\mu > 0$). Similarly, ammonia is a polar molecule made of polar bonds. The corresponding dipoles do not compensate each other ($\mu > 0$). On the other hand, CCl₄ is a nonpolar molecule made of polar bonds that do compensate each other ($\mu = 0$).

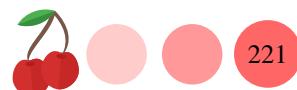


On one hand, each of the C—O bonds on the carbon dioxide molecule is a polar bond. However, CO₂ is a linear molecule and the polarity of each C—O bonds compensate so that at the end the molecule is polar.



Finally, in some molecules, the dipoles of different bonds can have different directions, partially compensating for each other, as shown below for the case of methanol (CH₃OH). The O—H dipole is larger than the C—O dipole as hydrogen is less electronegative (EN=2.2) than carbon (EN=2.5). Therefore both dipole moments reduce giving an overall dipole. Note the C—O—H bonds should be arranged in a bent geometry.

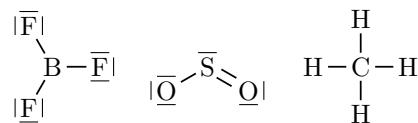


**Sample Problem 104**

Identify the polar character (polar/nonpolar) of the following molecules: BF_3 , SO_2 , and CH_4 .

SOLUTION

Let us analyze the geometries of the three molecules:



The bonds on SO_2 do not cancel out, as they do not point in opposite directions. Hence this molecule is polar. On the other hand, the bonds on methane and BF_3 cancel each other out, and hence even when the C-H and B-F bonds are polar, these two molecules would be non-polar.

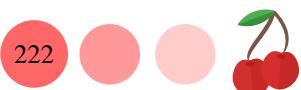
◆ STUDY CHECK

Identify the polar character (polar/nonpolar) of the following molecules: O_2 and NH_3 .

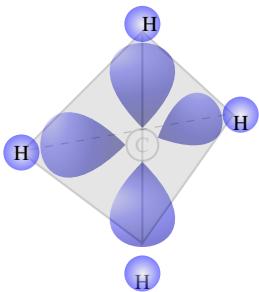
Polarity and mixing Polarity is a key property when two liquids or two gases mix. If the mixing molecules have the same polar character they will be able to mix, whereas they will not mix when the polar character is different. For example, H_2O and HCl mix well as both are polar molecules. Differently, H_2O and CCl_4 do not mix well, as while water is a polar molecule, carbon tetrachloride (or chloro methane) is a nonpolar molecule. Differences in polarity create immiscibility in liquids and gases. Finally, methanol (CH_3OH) is a polar molecule as well. The central atom of a molecule (C) is connected to three hydrogens and an OH group. Hence this will be a polar molecule as one of the atoms attached to carbon is different. Both molecules, water, and methanol will mix as they have the same polarity. As a general rule: molecules with the same polarity (polar-polar or nonpolar-nonpolar) will mix.

Molecules with the same polarity Methanol (CH_3OH) is a polar molecule as well. The central atom of molecule (C) is connected to three hydrogens and an OH group. Hence this will be a polar molecule as one of the atoms attached to carbon is different. Both molecules, water, and methanol will mix as they have the same polarity. Methane (CH_4) is a nonpolar molecule, as the four polar C-H bonds compensate each other. Similarly, CCl_4 , tetrachloro methene, is another nonpolar molecule, for the same reason. Both molecules, CH_4 and CCl_4 will mix together. As a general rule: molecules with the same polarity (polar-polar or nonpolar-nonpolar) will mix.

Molecules with different polarity CCl_4 is a nonpolar molecule, and H_2O is a polar molecule. As both have different polar characters they will not mix. If you mix water and CCl_4 , two phases will remain instead of a single mixed liquid phase. As a general rule: molecules with different polarity (polar-nonpolar) will not mix. Another example will be water and oil. Water is polar, and oil is a nonpolar molecule. As a consequence, these two molecules will not mix. Soap has a polar and nonpolar parts. To remove oil from water, soap helps mix both polar water and nonpolar oil.



9.4 Hybrid orbitals

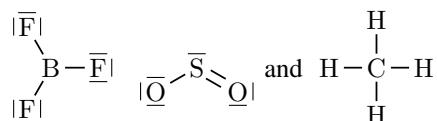


The molecular orbital theory is the most advanced bonding theory able to describe bond energies and bond lengths. Atomic orbitals are waves. When combining two waves one can obtain two possible results: a constructive combination and a destructive combination. The molecular orbital theory assumes that atomic orbitals combine to form molecular orbitals. For every two atomic orbitals you can obtain two possible molecular orbitals: one is called bonding orbital, resulting from the constructive combination, and another one is called antibonding orbital, resulting from the destructive combination. In this section, we will learn how to interpret molecular orbital diagrams.

From ABE code to hybridization To obtain the hybridization of an atomic center in a molecule we just need the ABE code and Table 9.6. For example, if the code of a molecule is AB_4 , the hybridization of the molecule will be sp^3 . Similarly, if the class is AB_3 the hybridization will be sp^2 and in this case, an empty p orbital will remain in the bond—mind there are three different p orbitals: p_x , p_y and p_z . Another example would be a molecule with class AB. In this case, the hybridization will be sp and two empty p orbital will remain in the bond. A final example would be a molecule with class AB_4E . This time, the hybridization would be sp^3d^2 . Mind that in general, the number of hybrid orbitals corresponds to adding the E and B from the class. For example, AB_4E_2 , we have two E and four B with a total of six orbitals, hence we will need a s , three p 's, and two d 's.

Sample Problem 105

Given the following Lewis structures, identify the hybridization of the central atom:

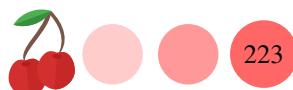


SOLUTION

In order to identify the hybrid character of the central atom, we first need to obtain the ABE code. For BF_3 the class is AB_3 , for SO_2 is AB_2E and finally for CH_4 is AB_4 . The number of electron regions for BF_3 is three. Therefore we would need three hybrid orbitals: sp^2 . An empty p orbital will remain unused in the bond. For SO_2 we need three electron regions and hence the hybridization of the central atom will also be sp^2 . For the case of methane, the hybridization will be sp^3 , as the molecule has four electron regions.

◆ STUDY CHECK

Identify the hybridization of the central atom for the following molecules: O_2 and NH_3 .

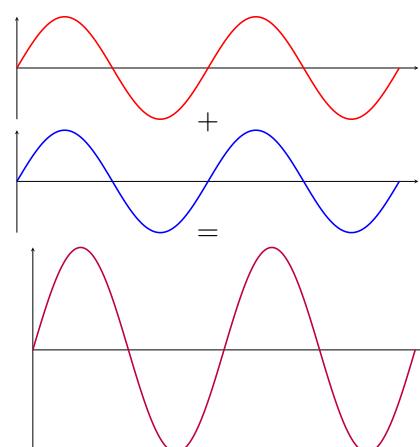
**Table 9.6 Equivalency between the ABE code and the orbital hybridization**

ABE Code	Electron Regions	Hybrid	Shape	Bond Angle
AB ₂ , ABE	2	sp		180°
AB ₃ , AB ₂ E, ABE ₃	3	sp ²		120°
AB ₄ , AB ₃ E, AB ₂ E ₂ , ABE ₃	4	sp ³		109.5°
AB ₅ , AB ₄ E, AB ₃ E ₂ , AB ₂ E ₃	5	sp ³ d		90° and 120°

9.5 Molecular orbital theory

Molecules consist of arrangements of atoms presented in different forms. Let us use as an example the H₂O molecule, which contains two hydrogen atoms and one oxygen. Knowing that both hydrogens are connected to oxygen through a covalent bond, one can envision several molecular geometries such as a linear geometry or maybe a v-shaped geometry with oxygen at the point. The geometry of a molecule determines its properties, and small geometrical changes can have severe consequences on the functioning of molecules. For example, at high temperatures, when proteins in the body denaturalize losing their unique structure they also lose their functionality. The goal of this section is to identify the approximate shape of a given molecule.

Bonding and antibonding orbitals Atomic orbitals (AOs) combine to produce molecular orbitals (MOs). The combination of two atomic orbitals results in two new molecular orbitals: a bonding orbital and an antibonding orbital. Bonding MOs are more stable than the corresponding atomic orbitals. Antibonding MOs are less stable—they have higher positive energy—than the corresponding AOs. Antibonding





orbitals are normally labeled with a * sign. Let us analyze both combinations of a $1s$ orbital. We can add both $1s$ orbitals and the result is a bonding orbital, or we can subtract both $1s$ orbitals and the result is an antibonding orbital, as the electron density cancels.

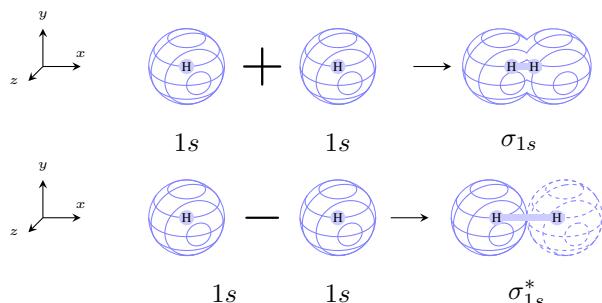
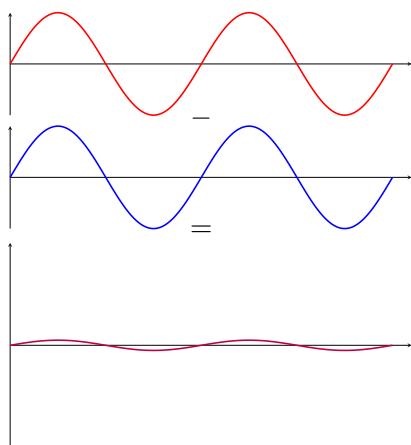


Figure 9.7 Bonding and antibonding σ orbitals resulting of combining two $1s$ atomic orbitals of Hydrogen.



Sigma and pi orbitals Let's analyze now the mixing of two $2p_x$ orbitals of two oxygen atoms to make an O_2 molecule. Mind that p orbitals look like dumbbells and each side of the dumbbell is called a lobe. In the p_x orbital the positive lobe is on the right side and the negative lobe on the left side. When combining both $2p_x$ if we add both orbitals we obtain a bonding orbital and if we subtract them we obtain an antibonding orbital. Both of these orbitals are called σ orbitals, as the lobes of the orbitals mixing go through the axes of the molecule being formed—the molecule is located in the X axis (see Figure 9.7). Differently, if we combine two $2p_y$ orbitals we will obtain two π orbitals, as the lobes of the molecular orbital is perpendicular to the axes of the molecule being formed (see Figure 9.8). The first orbital is bonding as both lobes overlap constructively, whereas the second orbital is antibonding as both lobes cancel out.

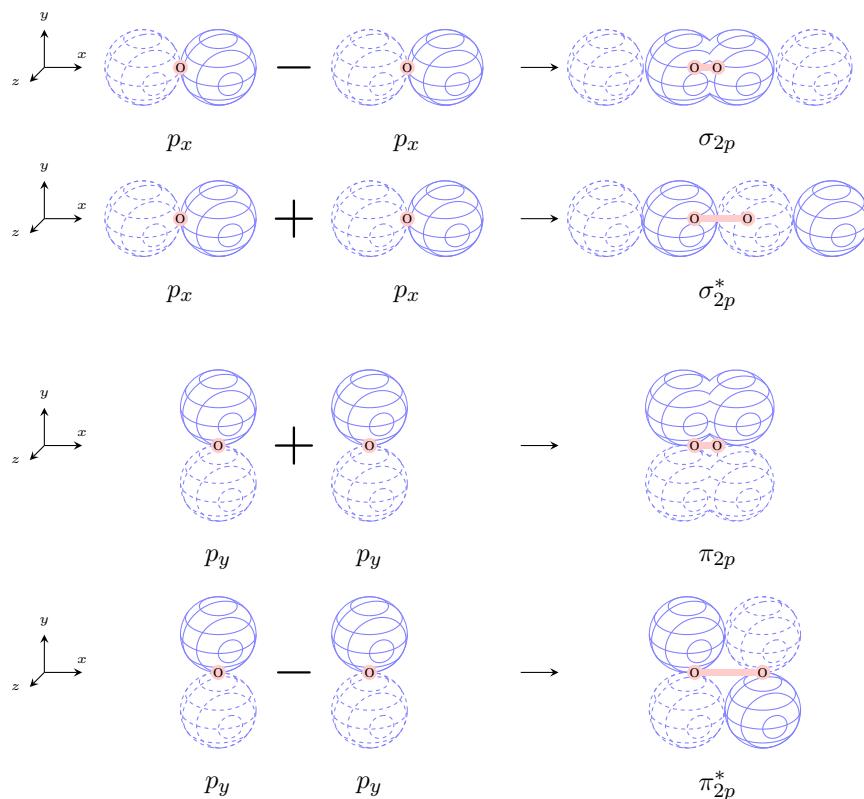
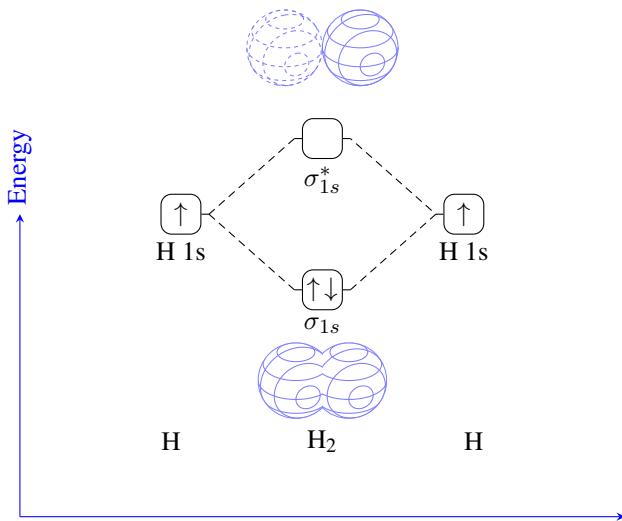
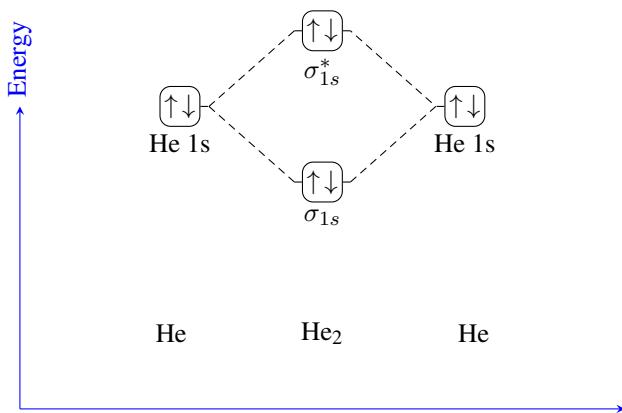


Figure 9.8 (Top) Bonding and antibonding σ orbitals resulting of combining two $2p_x$ atomic orbitals of Oxygen. (Bottom) Bonding and antibonding π orbitals resulting of combining two $2p$ atomic orbitals of Oxygen.

The case of molecular hydrogen Let us analyze the case of the formation of the H_2 molecule from two Hydrogen atoms. Each H atom has one $1s$ orbital. Therefore, according to the Molecular orbital theory, both orbitals will combine to produce two MO's. When you combine s atomic orbitals, the resulting MOs are always sigma. Sigma refers to the symmetry of the orbital. Therefore, the resulting MOs will be σ_{1s} and σ_{1s}^* . Each AO contains one electron, hence the set of MO's will also contain two electrons that will occupy the most stable σ_{1s} . The resulting MO diagram is below. In this diagram, the atomic orbitals of H are on the left and right, whereas the MO's are in the center. We can also give the MO configuration as $H_2 = \sigma_{1s}^2$. The hydrogen molecule is more stable than the separate hydrogen atoms. Why is that? the molecular orbitals of the molecule are lower in energy than the atomic orbitals of the hydrogen atoms. This means they have more energy—as energy is negative that also means they are more stable. That is the reason why the hydrogen molecule is a stable existing molecule and takes energy to break down this molecule into atoms.

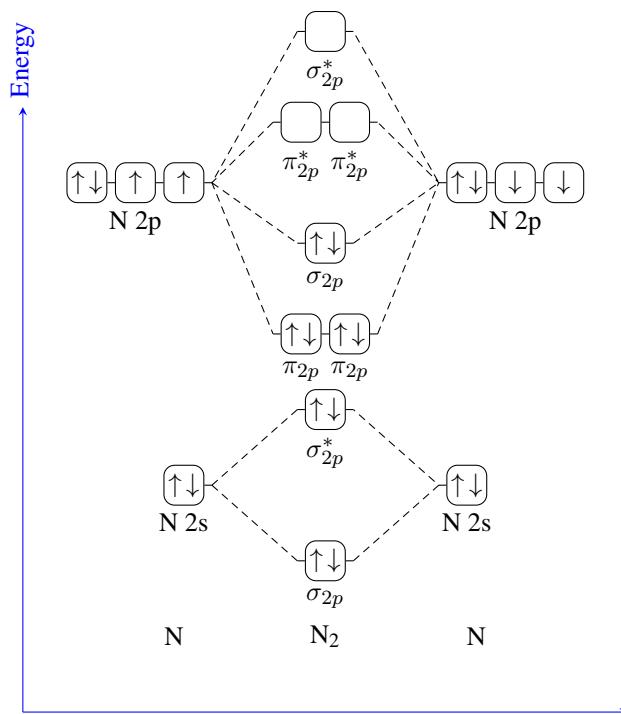


The case of molecular helium Let us analyze the case of the formation of the hypothetical Ne_2 molecule from two He atoms. Each He atom has one $1s$ orbital with two electrons. Therefore, according to the Molecular orbital theory, both orbitals will combine to produce two MO's with a total of four electrons. The resulting MOs will be as well: σ_{1s} and σ_{1s}^* . This time, MO configuration is: $He_2 = \sigma_{1s}^2 \sigma_{1s}^{*2}$. In general antibonding orbitals are not stable. In the He molecule we stabilize the molecule by forming two σ_{1s}^2 orbitals, but we also destabilize the molecule by forming σ_{1s}^{*2} . Hence the He_2 molecule will not be stable compared to the atoms:



From MO diagram to MO configuration Obtaining a MO diagram is not obvious, and these diagrams can only be obtained after very complicated quantum mechanics simulations. However, after the MO diagram is given, one can obtain the MO configuration. From this configuration, we can calculate two main properties: the bond order—related to the length of the molecule—and the magnetic character of the molecule. Let us use the case of N_2 : In this diagram, the lower MO's are the most stable and should be filled first. The higher MO are less stable and they are listed on the right side of the MO configuration. For example, the MO configuration of N_2 would be:

$$N_2 = \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$$



Bond order of a MO configuration Let us go back to the MO configuration for N_2 . In this configuration, we have some of the electrons occupying bonding MO and others occupying antibonding MO's. The bond order is just the number of bonding electrons—the number of electrons occupying bonding MO's—minus the number of antibonding electrons—the number of electrons occupying antibonding MO's—divided by two. The formula is:

$$BO = \frac{(n - n^*)}{2} \quad \text{Bond Order}$$

where:

n is the number of electrons occupying bonding MO's

n^* is the number of electrons occupying antibonding MO's

The bond order is related to the stability of the molecule and to the length of its chemical bond. The larger the bond order the most stable is the molecule as more electrons occupy bonding orbitals. The larger the bond order the smaller the chemical bond, and the atoms are looser.

Sample Problem 106

Given the following MO configurations: (a) $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^1$ and (b) $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2 \pi_{2p}^{*3}$. Calculate the bond order and compare the length of the chemical bond of both molecules.

SOLUTION

The bond order is the number of bonding electrons minus the number of antibonding electrons divided by two. For the first example, we have seven bonding electrons and two antibonding. Hence the bond order will be 2.5. For the second example, we have eight bonding electrons and five antibonding. Hence the bond order will be 1.5. The larger the BO the smaller the bond, hence the second molecule has a smaller bond.


◆ STUDY CHECK

Calculate the bond order for $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$.

Paramagnetism and diamagnetism One of the uses of the MO configuration is to predict the magnetic character (magnetic or non-magnetic) of a molecule. By reading the MO configuration of a molecule, we can also predict its magnetic character and hence estimate its magnetic properties. Paramagnetic molecules (normally referred to as magnetic) are attracted by magnetic fields, whereas diamagnetic molecules (normally referred to as non-magnetic) are repelled by magnetic fields. The magnetic character results from the presence of unpaired electrons in the MO configuration. For example $\sigma_{2s}^2 \sigma_{2s}^{*1}$ is a paramagnetic (magnetic) molecule as we have one unpaired electron in the σ_{2s}^* orbital. In contrast, $\sigma_{2s}^2 \sigma_{2s}^{*2}$ is a diamagnetic (non-magnetic) molecule, as it has no unpaired electrons.

Sample Problem 107

Given the following MO configurations, predict the magnetic character: (a)

$\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^1$ and (b) $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2 \pi_{2p}^{*3}$.

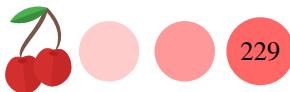
SOLUTION

The first example has an unpaired σ electron and hence it is paramagnetic. The second base also has a single unpaired electron, this time in the π_{2p}^* orbital. Mind π orbitals have capacity of four and hence can place two separate pairs of electrons.

◆ STUDY CHECK

Given the following MO configurations, predict the magnetic character: (a)

$\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$ and (b) $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2 \pi_{2p}^{*2}$.



CHAPTER 9

ELECTRON-DOT STRUCTURES OF MOLECULES

9.1 Indicate the number of bonds that can the following atoms form: (a) An atom with electron configuration ns^2np^4 (b) C (c) An atom with electron configuration ns^2np^2 (d) An atom with electron configuration ns^2np^1 (e) N (f) H

9.2 Indicate the number of bonds that can the following atoms form: (a) An atom with electron configuration ns^1 (b) An atom with electron configuration ns^2np^3 (c) O (d) An atom with electron configuration ns^2np^5 (e) P (f) B

9.3 Draw electron-dot structures for the following diatomic molecules that obey the octet rule: (a) F_2 (b) Cl_2

9.4 Draw electron-dot structures for the following diatomic molecules that obey the octet rule: (a) HF (b) HCl

9.5 Draw electron-dot structures for the following diatomic molecules that obey the octet rule: (a) ICl (b) HI

9.6 Draw electron-dot structures for the following diatomic molecules: (a) CO (b) N_2 (c) O_2

9.7 Draw electron-dot structures for the following molecules that obey the octet rule, given that the first atom listed is the central atom: (a) CHN (b) CO_2



9.8 Draw electron-dot structures for the following molecules that obey the octet rule, given that the first atom listed is the central atom: (a) CH₄ (b) CH₃Cl (c) OH₂

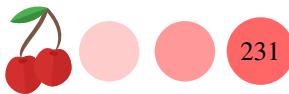
9.9 Draw electron-dot structures for the following molecules that obey the octet rule, given that the first atom listed is the central atom: (a) NH₃ (b) NCl₃

9.10 Draw electron-dot structures for the following molecules that obey the octet rule, given that the first atom listed is the central atom: (a) SeCl₂ (b) CH₂O

9.11 Draw electron-dot structures for the following molecules given that the first atom listed is the central atom. Some of the atoms might not obey the octet rule. If the species has a charge indicate the location of the charge: (a) BH₃ (b) BH₂F (c) POCl₃ (d) ClO₄⁻

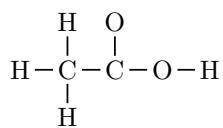
9.12 Draw electron-dot structures for the following molecules given that the first atom listed is the central atom. Some of the atoms might not obey the octet rule. If the species has a charge indicate the location of the charge: (a) BeH₂ (b) PCl₅ (c) SF₄ (d) ClF₃

9.13 Draw electron-dot structures for the following molecules given that the first atom listed is the central atom. Some of the atoms might not obey the octet rule. If the species has a charge indicate the location of the charge: (a) I₃⁻ (b) Br₃⁻ (c) SF₆

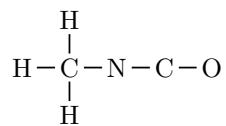


9.14 Draw electron-dot structures for the following molecules given that the first atom listed is the central atom. Some of the atoms might not obey the octet rule. If the species has a charge indicate the location of the charge: (a) ClF₅ (b) XeF₄

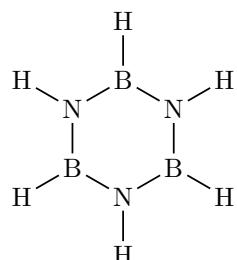
9.15 Given the skeletal structure below, draw the lewis structure of the molecule:



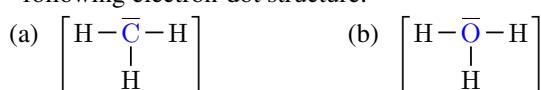
9.16 Given the skeletal structure below, draw the lewis structure of the molecule:



9.17 Given the skeletal structure below, draw the lewis structure of the molecule:

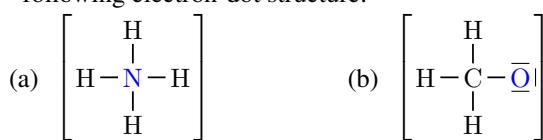


9.18 Indicate the charge of the atom marked blue in the following electron-dot structure:





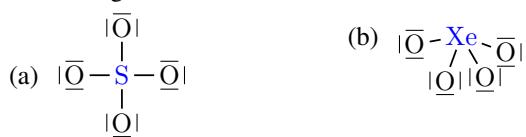
9.19 Indicate the charge of the atom marked blue in the following electron-dot structure:



9.20 Indicate the charge of the atom marked blue in the following electron-dot structure that follow the octet rule:



9.21 Indicate the charge of the atom marked blue in the following electron-dot structure that follow the octet rule:



MOLECULAR SHAPE

9.22 Identify the molecular shape of the molecules:

(a) NH₃ (b) CH₄

9.23 Identify the molecular shape of the molecules:

(a) H₂ (b) BeCl₂ (c) BF₃

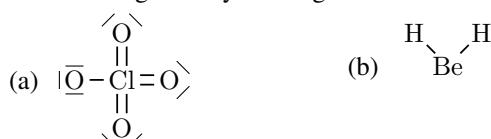
9.24 Given the following Lewis structures, predict the molecular geometry and angles:



9.25 Given the following Lewis structures, predict the molecular geometry and angles:



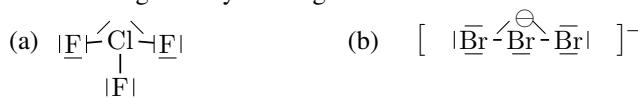
9.26 Given the following Lewis structures, predict the molecular geometry and angles:



9.27 Given the following Lewis structures, predict the molecular geometry and angles:



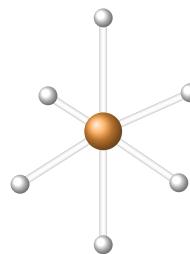
9.28 Given the following Lewis structures, predict the molecular geometry and angles:



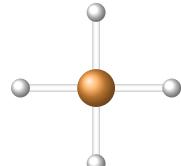
9.29 Given the following Lewis structures, predict the molecular geometry and angles:



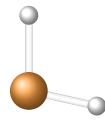
9.30 Identify the name of the following molecular structure:



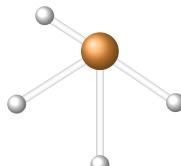
9.31 Identify the name of the following molecular structure:



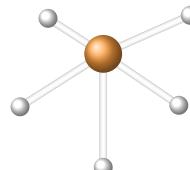
9.32 Identify the name of the following molecular structure:



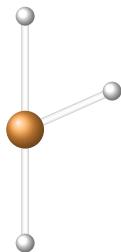
9.33 Identify the name of the following molecular structure:



9.34 Identify the name of the following molecular structure:



9.35 Identify the name of the following molecular structure:



POLARITY

9.36 Describe the trend in electronegativity (increases, decreases): (a) from Na to Mg (b) from Cs to Ba (c) from S to O (d) from P to C (e) from K to Rb (f) from B to C (g) from Li to Na

9.37 Describe the trend in electronegativity (increases, decreases): (a) from S to Cl (b) from Se to Br (c) from Rb to Cs (d) from P to O (e) from Cl to F (f) from Li to Be (g) from Se to Cl

9.38 Arrange the atoms in the following set in order of increasing electronegativity: (a) Li, Be, and B (b) Rb, Na, and K (c) N, C, and B

9.39 Arrange the atoms in the following set in order of increasing electronegativity: (a) P, Cl, and S (b) Br, F, and Cl (c) S, O, and Se

9.40 Classify the following bonds as ionic, polar covalent and nonpolar covalent by calculating the electronegative difference: (a) S–P (b) O–Mg (c) H–Na (d) H–N (e) Na–Cl (f) S–C

9.41 Classify the following bonds as ionic, polar covalent and nonpolar covalent by calculating the electronegative difference: (a) H–K (b) H–Li (c) O–Li (d) O–Na (e) Na–F (f) S–H

9.42 For the following ionic bonds indicate the positive and negative end of the dipole and whether the resulting dipole points to the left or to the right: (a) F—K (b) Se—Rb (c) Na—Cl

9.43 For the following ionic bonds indicate the positive and negative end of the dipole and whether the resulting dipole points to the left or to the right: (a) S—Ca (b) K—Br (c) Mg—S

9.44 For the following covalent bonds indicate the partially positive and negative end of the dipole and whether the resulting dipole points to the left or to the right: (a) C—F (b) N—F (c) Si—O (d) Br—S

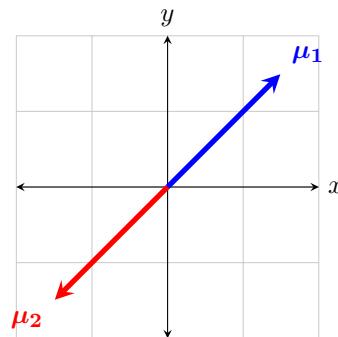
9.45 For the following covalent bonds indicate the partially positive and negative end of the dipole and whether the resulting dipole points to the left or to the right:

(a) N—O (b) S—C (c) N—C (d) Si—B

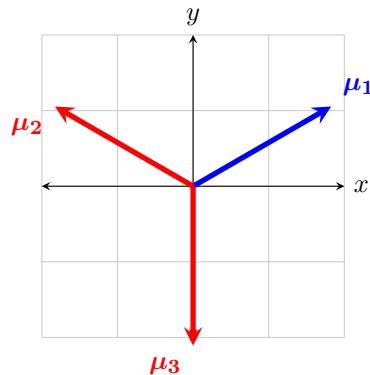
9.46 Select the more polar bond from the following set of bond pairs: (a) N–O or N–P (b) P–Si or P–S (c) S–Cl or S–Se

9.47 Select the more polar bond from the following set of bond pairs: (a) H–O or H–F (b) O–S or S–Se (c) H–Cl or H–F

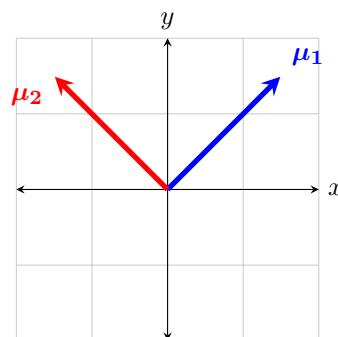
9.48 Predict if the following dipole distribution will lead to an overall dipole moment:



9.49 Predict if the following dipole distribution will lead to an overall dipole moment:

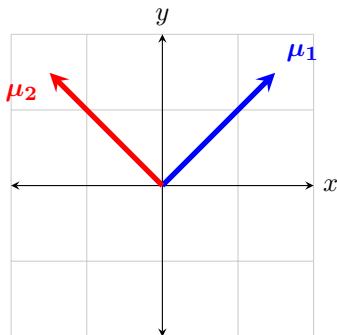


9.50 Predict if the following dipole distribution will lead to an overall dipole moment:

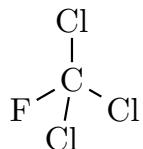




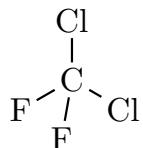
9.51 Predict if the following dipole distribution will lead to an overall dipole moment:



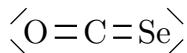
9.52 Predict if the following bond arrangement will lead to an overall dipole moment:



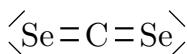
9.53 Predict if the following bond arrangement will lead to an overall dipole moment:



9.54 Predict if the following bond arrangement will lead to an overall dipole moment:



9.55 Predict if the following bond arrangement will lead to an overall dipole moment:



9.56 Indicate the polar character (polar, nonpolar) of the following molecules: (a) H₂O (b) HCl (c) CO₂ (d) CO (e) PF₃ (f) SiCl₄

9.57 Indicate the polar character (polar, nonpolar) of the following molecules: (a) CF₄ (b) NH₃ (c) SeF₂ (d) O₂ (e) CH₄ (f) H₂

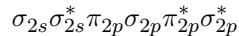
HYBRID ORBITALS

9.58 Indicate the hybridization of: (a) NH₃ (b) CH₄ (c) H₂O

9.59 Indicate the hybridization of: (a) NH₃ (b) CH₄ (c) H₂O

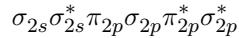
MOLECULAR ORBITAL THEORY

9.60 Using the MO order provided below



obtain the MO configuration for: (a) B₂ (b) C₂

9.61 Using the MO order provided below



obtain the MO configuration for: (a) O₂ (b) F₂⁺

9.62 Indicate the magnetic (paramagnetic or diamagnetic) configuration of the molecule with MO configuration: $\sigma_{2s}^2\sigma_{2s}^{2*}\sigma_{2p}^2\pi_{2p}^4\pi_{2p}^{3*}$

9.63 Indicate the magnetic (paramagnetic or diamagnetic) configuration of the molecule with MO configuration: $\sigma_{2s}^2\sigma_{2s}^{2*}\sigma_{2p}^2\pi_{2p}^4\pi_{2p}^{2*}$

Ch. 10. Solids and liquids

HERE are three different states of the matter: solid, liquid and gas. At this point, we have studied the properties of gases and liquid solutions. We have not encountered yet solids or pure liquids. This chapter fully deals with the properties of solids and liquids. Liquids have indeed very peculiar properties and this chapter will cover—among others—the vapor pressure. Liquids are not isolated; they are normally in contact with the atmosphere. The liquid molecules which are closer to the air can escape forming a vapor; this vapor exerts certain pressure. This vapor is what you feel, for example, when the weather is very humid. Finally, this chapter covers the idea of intermolecular forces. The molecules of an ideal gas are independent of each other. This means they do not see each other at all—they do not interact with each other. Differently, the molecules of liquids and solids interact with each other through stronger forces that act between molecules—these are called intermolecular forces. The properties of these forces will help you understand why some liquids boil at higher temperatures than others or some solids have higher melting points.

10.1 Intermolecular forces

Atoms in liquid or solid compounds are connected through chemical bonds, and bonds are forces within molecules. These bonds can be ionic or covalent depending on the nature of the elements that form the molecule. At the same time, the molecules of a liquid or solid compound interact with each other through intermolecular forces. The word intermolecular means between molecules. This section describes the three existing types of intermolecular forces as well as their nature and intensity.

Intermolecular forces and intramolecular interactions

Molecules are made of atoms that connect through *intramolecular* interactions such as covalent or ionic bonds. Differently, molecules interact with each other through *intermolecular* interactions. The prefix *inter* means "occurring between", whereas the prefix *intra* means "occurring within". Intermolecular forces are responsible for the melting and boiling point of a chemical. On one hand, the stronger the forces the higher the melting and boiling point. On the other hand, the more intermolecular interactions the higher the melting and boiling point. This is because to melt or boil a chemical we need to overcome the intermolecular forces that connect molecules to release them into a different state of matter. In the following, we will describe the three main types of intermolecular forces (some books describe four types of intermolecular forces counting the ion-molecule interaction).

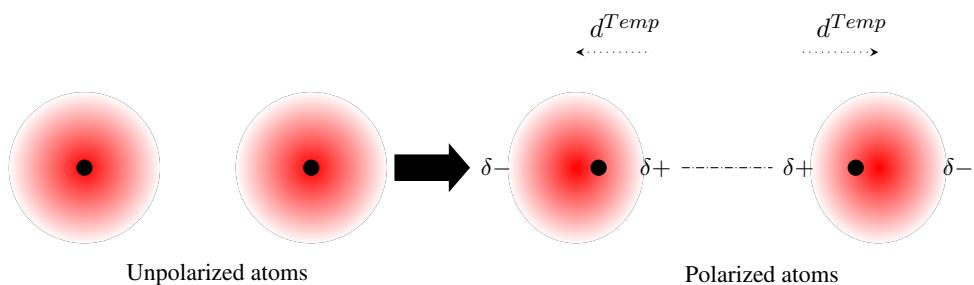


Figure 10.1 Dispersion forces result from instantaneous dipole moments resulting from the polarization of the electron density of atoms and molecules.

Dispersion forces All molecules are made of atoms that contain electrons. The electron density of an atom is distributed homogeneously without uneven charge distributions. As a consequence, atoms in general have no permanent dipole moment without negatively or positively charged regions. Still, when two atoms get close together, the presence of each other affects their electron density creating temporary dipole moments. We call this effect polarizability. This temporary dipole is responsible for London dispersion forces, also called Van der Waals forces or simply dispersion forces. Dispersion forces exist in all chemicals, as all chemicals can be polarized. The larger the atomic number, or the molar weight of the compound, the stronger these forces are. This is because in general the larger the atomic weight the more polarizable atoms are, and hence, they tend to generate stronger temporary dipoles, produced from charge polarization.

The melting (or freezing) and boiling points of the noble gases are given in the Table below, where you can see how the larger the atomic mass of the gas the higher the melting—and boiling points. Mind that normally, the melting and freezing points of a substance are the same. Dispersion forces are common in chemicals made of hydrogen and carbon—we call these compounds hydrocarbons. The larger the size of the molecule the larger the effects of dispersion forces. For example:

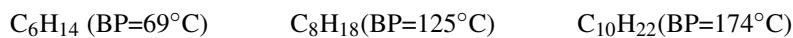


Table 10.1 Freezing and boiling point of the noble gases

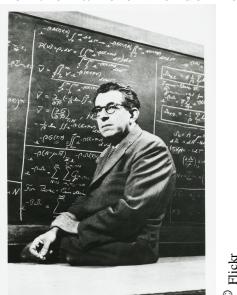
Gas	Atomic Weight (amu)	Melting Point (°C)	Boiling Point (°C)
He	2	—	4
Ne	10	25	27
Ar	18	84	87
Kr	36	116	121
Xe	54	162	167
Rn	6	202	211

Dipole-Dipole forces Atoms have different electronegativity that is, a different tendency to attract the electron density in a bond. In the periodic table, electronegativity increases going from left to right and top to bottom. Elements in the top right of the table (Cl, F) tend to be very electronegative and hence they tend to strongly attract the electrons on chemical bonds. Differently, elements on the bottom left part of the table are electropositive and they tend to give away the electrons in the bond. Dipole

▼ Polymer molecules interact by means of dispersion



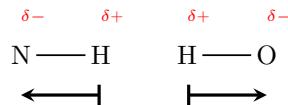
▼ Fritz London a german physicist is responsible for the name of London forces



▼ geckos stick because of the van der Waals force



moments result from differences in electronegativity. When an electronegative atom is connected to an electropositive atom in a bond, the electronegativity difference creates permanent dipole moments, and molecules with permanent dipole moments are called polar molecules. The dipole moment of a bond is a vector that points from the most electropositive atom to the most electronegative atom. For example for the O-H and N-H bonds,



As such, the molecule HCl would be polar as a result of the combination of an electropositive atom (H) and an electronegative atom (Cl). Similarly, HF would be a polar molecule too. Dipole-dipole forces exist only in polar compounds, being the result of permanent dipole moments. These types of interactions are stronger than dispersion forces but weaker than normal interatomic covalent bonds. Molecules with dipole moment can attract each other through dipole forces, orienting themselves so that their positive side aligns with the negative side maximizing the electrostatic attraction. At the same time, dipole forces depend on the distance and at large distances are less effective. The dipole moment of a molecule is measured in Debye (D). For example, the dipole moment of HCl is 1.05D, whereas the dipole moment of HF is 1.82D. The stronger the dipole moment the stronger the dipole-dipole interactions. For example, when comparing C₃H₈ and CH₃OCH₃, the former has an almost null dipole moment, whereas the latter has a dipole moment of 1.3D. The boiling point of C₃H₈ is -42°C whereas the boiling point of CH₃OCH₃ is -25°C. The table below lists some dipole moments and boiling points showing the trend that the larger the dipole moment the higher (more positive) the boiling point.

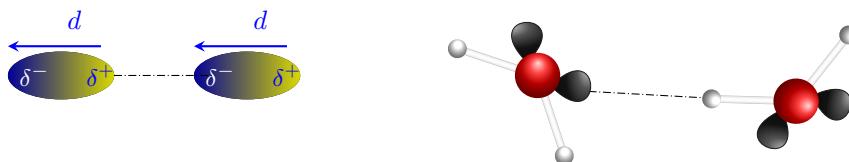


Figure 10.2 (Left) Dipole-dipole forces result from the interaction of permanent dipole moments existing in polar molecules. (Right) two water molecules interacting by means of hydrogen bonds

Table 10.2 Boiling (BP) point of a series of hydroacids

Compound	Dipole moment (Debyes)	Boiling Point (°C)
C ₃ H ₈	0.1	-42
CH ₃ OCH ₃	1.3	-25
CH ₃ Cl	2.0	-24
CH ₃ COH	2.7	-21
CH ₃ CN	3.9	-82

Hydrogen bonds Hydrogen bonds are the strongest of all intermolecular forces and exist only in molecules containing very specific bonds; in particular, they only exist in molecules containing H–F, H–N, or H–O bonds. An example of a molecule with hydrogen bonds is HF or NH₃. Hydrogen bonds are a specific type of dipole-dipole interaction responsible, among others, for



some of the high boiling points of water. Due to the existence of hydrogen bonds water is liquid at room temperature (H_2O , BP=100°C), in comparison with similar molecules (H_2S , BP=-60°C). The anomalous character of oxygen, fluorine, and nitrogen results from the fact that these are very electronegative elements with lone pairs of electrons—these are non-bonding pairs of electrons—that enable the creation of hydrogen bonds. In particular, oxygen has two lone pairs, nitrogen one and fluorine three. The combination of high electronegativity, the presence of lone pairs, and the presence of hydrogen atoms makes hydrogen bonds possible.

Sample Problem 108

Indicate what types of intermolecular forces exist in the following molecules:

	HCl	CH_4	H_2O	CH_3Cl
Dispersion				
Dipole-				
Dipole				
H-bonds				

SOLUTION

All molecules can interact by means of dispersion forces. Differently, only polar molecules can interact by means of dipole-dipole forces. Finally, only molecules with a H–F, H–N or H–O bond can interact by means of hydrogen bonds. For these reason, from the table only HCl, H_2O and CH_3Cl has dipole forces, and only H_2O has hydrogen bonds.

	HCl	CH_4	H_2O	CH_3Cl
Dispersion	✓	✓	✓	✓
Dipole-	✓	✗	✓	✓
Dipole				
H-bonds	✗	✗	✓	✗

◆ STUDY CHECK

Indicate what types of intermolecular forces exist in the following molecules: NH_3 , HF, and CH_3-CH_3 .

Intermolecular forces of liquids and boiling Boiling a liquid requires energy. This energy is invested in separating the molecules from the liquid until they are spread apart. To separate the molecules of a liquid, we need to overcome intermolecular forces. Imagine boiling CH_4 . We know the molecules of methane only interact among themselves through weak dispersion forces. Imagine now boiling water. Water is polar and water has O–H bonds, hence water molecules interact through dispersion, dipole-dipole, and hydrogen bonds. The energy needed to separate the molecules of water will be larger than the energy required to separate the molecules of methane. The more intense the intermolecular forces, the higher the boiling point. Also, the more types of intermolecular forces present in a liquid the higher the boiling point. Finally, we can apply these ideas not only to liquids but also to solids.

Sample Problem 109

Compare the boiling point of these two molecules: HCl and H₂O.

SOLUTION

Let us build a table with the different types of intermolecular forces present in each liquid. The molecules of both liquids can interact by means of dispersion forces and also dipole-dipole forces, as both are polar molecules. Differently, only molecules with a H–F, H–N or H–O bond can interact by means of hydrogen bonds. For these reason, H₂O liquid contains hydrogen bonds.

	HCl	H ₂ O
Dispersion	✓	✓
D-D	✓	✓
H-bonds	✗	✓

Hence, water will boil at a higher temperature.

❖ STUDY CHECK

Compare the boiling point of these two molecules: CH₃F and CH₄.

▼ Cooking salt, NaCl is a crystalline solid



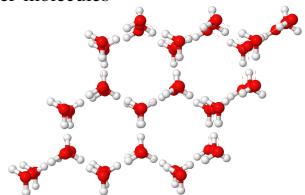
© Wikipedia

▼ SiO₂ is an amorphous solid



© Wikipedia

▼ Ice, H₂O(s) is a molecular solid made of water molecules



© Wikipedia

▼ Gold is an atomic solid made of gold atoms.



© Wikipedia

10.2 The solid state

What makes solids unique in comparison to liquids and gases? They answer is their structure. There are two main different types of solids: crystalline solids and amorphous solids. Crystalline solids are made of atoms or molecules periodically, regularly, arranged in the three dimensions of the space. Examples of a crystalline solid are table salt or sugar. Amorphous solids have disordered structures. An example of an amorphous solid is window glass. This section will focus on the properties of crystalline solids as their periodicity makes their properties easier to study.

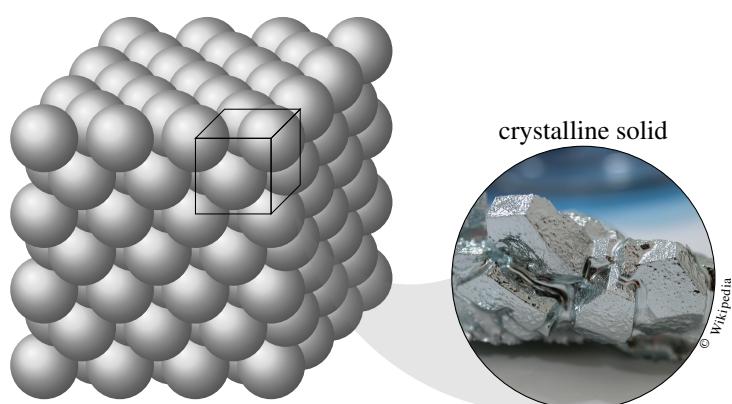


Figure 10.3 Unit cell of a solid of a crystalline solid. The whole structure of the solid results from the replication of a unit cell and just this unit cell is necessary to characterize the structure of the solid.

Crystalline lattice: the unit cell The structure of crystalline solids is periodic. The term does not refer to periodic in time, but in periodic in space. Hence,



the structure of crystalline solids is the result of the repetition of a small piece of the structure in the space. The overall structure is called *crystalline lattice*. Here an example of a very simple two dimensional lattice. In this lattice, the central box is repeated infinitely in two directions of the space generating a lattice. As the lattice is made of repetition, the smallest repeating unit is called the *unit cell*. Therefore, simply with the unit cell one can generate the whole crystal lattice by repeating the unit cell in the three dimensions. Therefore, it is unnecessary to study the crystalline whole lattice as the unit cell is enough to understand many properties of crystalline solids such as their density. In the following we will study in more detail the properties of crystalline solids and some of the most common unit cells.

Types of crystalline solids Examples of crystalline solids are: sugar and table salt. These two solids have very different constitutions. Table salt is made of ions: Na^+ and Cl^- . Sugar is made of molecules. We say NaCl is an ionic solid, whereas sugar is a *molecular solid*. Other examples of *ionic solids*: MgO , CaF_2 . Other examples of *molecular solids*: ice which is made of water molecules. A third type of crystalline solids are called *atomic solids*, as they are made of atoms. Think of metallic iron or graphite. Both are atomic solids made of atoms, Fe and C. Overall, molecular solids are made of molecules—often times covalent molecules—whereas ionic solids are made of ions and result from ionic compounds. Finally, atomic solids are made of atoms. In the following we will study more about a specific type of atomic solids: metallic solids. Metallic solids are indeed atomic solids made of metallic elements, such as for example gold ($\text{Au}_{(s)}$).

Sample Problem 110

Classify the following solids as ionic, molecular or atomic: diamond, dry ice (CO_2), iron and CaF_2 .

	diamond	CO_2	Fe	CaF_2
Molecular				
Ionic				
Atomic				

SOLUTION

In general ionic solids correspond to ionic compounds and molecular solids correspond to covalent compounds. Therefore, dry ice should be a molecular solid and CaF_2 and ionic solid. Iron and diamond are both made of atoms and hence they are atomic compounds.

	diamond	CO_2	Fe	CaF_2
Molecular	✗	✓	✗	✗
Ionic	✗	✗	✗	✓
Atomic	✓	✗	✗	✗
Metallic	✗	✗	✓	✗

◆ STUDY CHECK

Classify the following solids as ionic, molecular or atomic: silver, graphite, CaCO_3 and $\text{NH}_3(s)$.

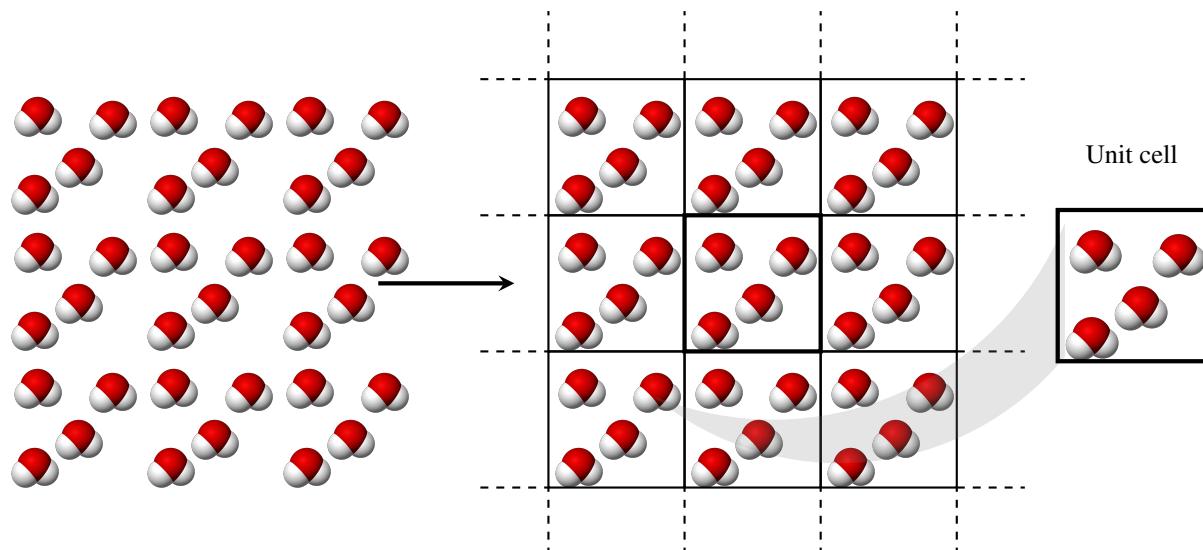


Figure 10.4 A periodic structure made of water molecules. The unit cell on the left contains four water molecules. The repetition of the unit cell, on the right, generates a two-dimensional structure.

10.3 Metals and ionic solids

Among the different types of crystalline solids, metals and ionic solids are very important. This section will cover the structure of metallic solids like gold or iron and ionic solids like sodium chloride.

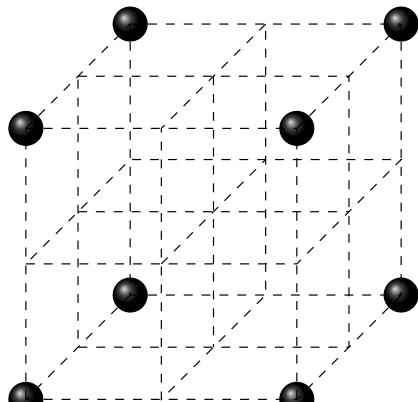
Closed packing of metals Metallic solids result from the packing of metal atoms in space. Picture a single layer of spheres all packed together. The most compact way to pack a layer of spheres is the situation in which one sphere is surrounded by six other spheres (layer A). This is called the closest packing. In this situation, every three spheres are connected by means of an indentation or dimple. Now let us think about how to pack a second layer on top of the first later. We can simply place the second layer just on top of the first layer (called layer A also). This would lead to a simple cubic packing arrangement (AA packing) which is not the most compact packing arrangement and the unit cell resulting from this packing is called *simple cubic*. Differently, we could pack the second layer on the indentations of the first layer, which would lead to more complex packing schemes as we try to add a third layer. There would be two possible ways to add a third layer of atoms. You can locate the third layer on top of the first layer leading to an ABA packing, with a resulting unit cell called *hexagonal close cell*, (*hcp*). Or you can locate the third layer on top of the indentations of the second layer leading to a ABC layer packing leading to a unit cell called *face centered cubic*, (*fcc*).

Table 10.3 (Left side) atoms per cell for each unit cell; (Right side) Sharing factor for each cell location

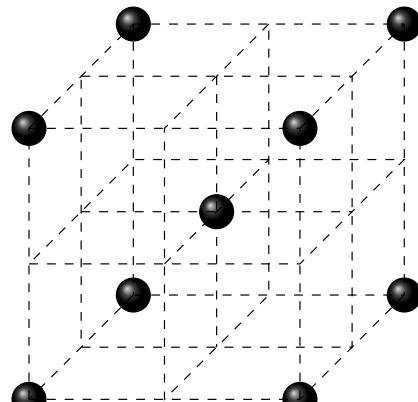
Structure	Atoms per cell	Cell location	Sharing factor, f
sc	1	Inside	1
bcc	2	Vertex	1/8
fcc	4	Face	1/2
		Edge	1/4



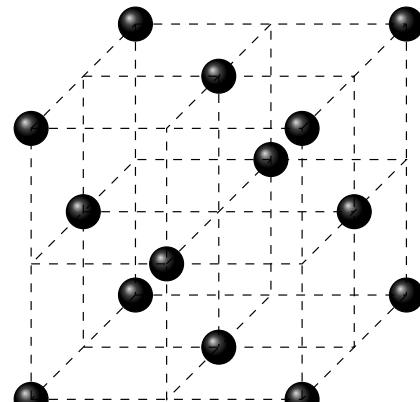
Atom sharing in unit cells Before we cover the different metallic units cells let us talk about atom sharing. Think about a cubic unit cell, that is a cube with one sphere (atom) in every corner of the cube. The whole lattice is produced by repeating the unit cell on the three dimensions. Hence, every corner of the cube is shared among other corners. This means, every corner-containing an atom—shares that atom with all units cells connected to that corner. Therefore, those atoms in the corner are not whole part of a single unit cell and they are shares. Every corner of a cube is shared among eight other cubes. Imagine piling numerous boxes in layers. Every corner of each box is shared by three other boxes in the same plane and by four boxes on the plane on top—that is a total of eight boxes. They way you need to think of the different atoms in a single unit cell, is that they are shared depending on their location. As we discussed, corners of a cubic unit cell are shared by a total of 8 others unit cells. Atoms that belong to a face of a unit cell are shared by two unit cells. Atoms that are inside a unit cell fully belong to a single unit cell and they are not shared. Atoms that belong to a edge of the cube—an edge is the line that connects two vertexes of a cube—are shared by four units cells.



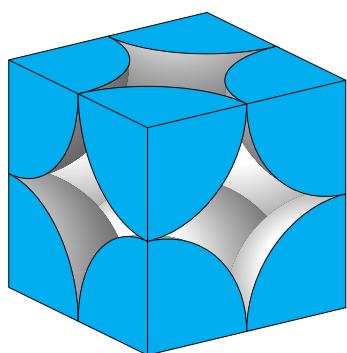
SCC (Simple cubic cell)



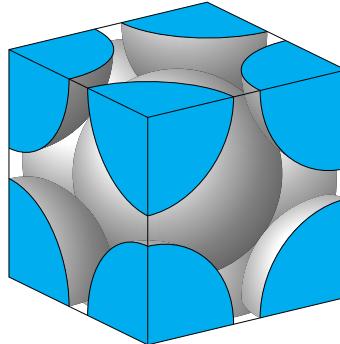
BCC (Body-centered cubic cell)



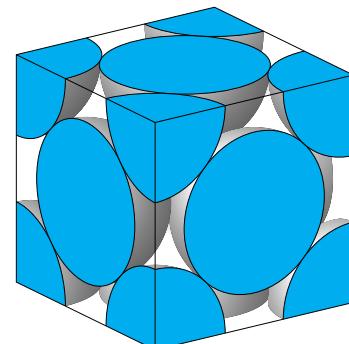
FCC (Face-centered cubic cell)



$$c = 2r$$

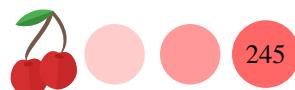


$$c = \frac{4}{\sqrt{3}}r$$



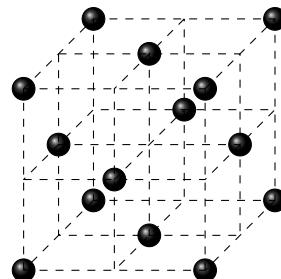
$$c = \sqrt{8}r$$

Figure 10.5 The different unit cells. Space-fill structures are shown on the bottom. The simple cubic unit cells have atoms in the corners of the cell. The body-centered cubic unit cell have atoms in the corners and one atom in the center. The face-centered unit cell has atoms in the corners and in the faces. The relationship between the cell parameter (c) and the atomic radius (r) is also given for each unit cell.



Sample Problem 111

The following structure is called face centered unit cell. This is a cubit unit cell with one atom in each corner of the cell and atoms also in the facets of the cell. Calculate the number of atoms in the unit cell:

**SOLUTION**

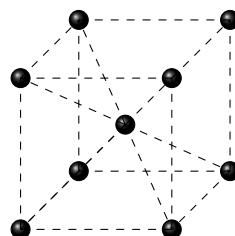
If you count the number of spheres in the drawing you might think the cell contains fourteen atoms. However, this is not true, as each sphere is shared by other unit cells. Remember each location of the unit cell counts as a fraction. If an atom is fully inside in the cell—not in the vertexes, neither in the faces or sides—the sharing factor is one. If an atom belongs to a vertex, the sharing factor is $1/8$. Atoms in a face has a sharing factor of $1/2$ and atoms in the edges have a sharing factor of $1/4$.

Location	Sharing Factor, f	# atoms, N	$f \times N$
Corner	$1/8$	8	1
Faces	$1/2$	6	3

By multiplying the number of atoms in each location by the sharing factor and adding we obtain the total number of atoms in the cell. Overall, this unit cell has four atoms:

◆ STUDY CHECK

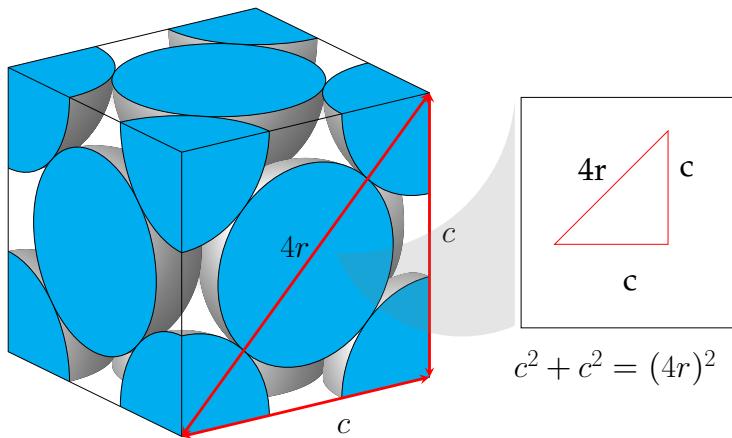
The following structure is called simple body centered unit cell. This is a cubit unit cell with one atom in each corner of the cell and an atom also in the center of cell. Calculate the number of atoms in the unit cell:



Metal unit cells Here we will cover three different metal unit cells, all cubic cells. First, the simple cubic unit cell, with an atom each of the vertexes of the cell. This is the less compact unit cell with one atom per unit cell. Second, the body-centered unit cell is a cubic unit cell with atoms in the vertex of the cell and a single atom in the center of the cell. This cell has two atoms per unit cell. Third, the face-centered unit cell, with atoms in the vertex of the cell and also on the faces of the cell, on the sides of the cube. This is the most compact unit cell, with four atoms per cell. In the following image you can manipulate a face-centered cubic cell.

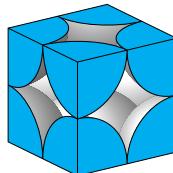


Cell parameter Cubic unit cells have the shape of a cube and hence all side of the cube have the same length. This length is called cell parameter c . Unit cells with large cell parameter have more spacing between atoms. The opposite is true for cells with smaller cell parameter. The cell parameter of a unit cell is related to the atomic radius. Let us analyze the case of a face-centered unit cell. In each side of the cell, in each face, we have four atoms in the vertexes and one in the center of the face. Of course these atoms do not belong only to this unit cell. However, if we symbolically cut the atoms in the face we can see the relation between the radius of the atom and the unit cell. The edges of the cell does not correspond to any cell parameter. However, the line that connect the bottom part with the opposite top part corresponds to a specific number of cell parameters, as the atoms are touching in this direction. In particular this distance is $4r$. Using Pythagoras theorem we have: $c^2 + c^2 = (4r)^2$. Therefore, $c = \sqrt{8}r$.



Sample Problem 112

For the following unit cell, calculate the relationship between the cell parameter and the atomic radius.

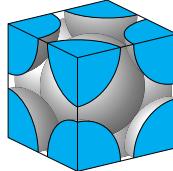


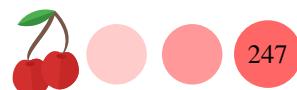
SOLUTION

For this unit cell, the atoms in the bottom part are touching. Hence, the cell parameter should be related to the atomic radius. In particular, two half atoms occupy the same distance as the cell parameter, so $c = r$.

◆ STUDY CHECK

For the following unit cell, calculate the relationship between the cell parameter and the atomic radius.





Metal density Different metals have different density. The value for density will depend on the cell parameter but also on the compacity of the unit cell, the more compact the unit cell the more atoms per cell and hence the more density. The formula that relates density with cell parameter and atoms per cell is:

$$d = \frac{N \cdot AW}{c^3 \cdot 6.023 \times 10^{-7}}$$

Metallic density formula

where:

d is the density in $g \cdot ml^{-1}$

N is the number of atoms per unit cell

6.023×10^{-7} is related to the conversion between atoms and grams

AW is the atomic weight of the metal

c is the cell parameter in pm

Sample Problem 113

Calculate density of iron ($AW = 55.845 g \cdot mol^{-1}$) knowing this is a bcc metal with cell parameter is 286pm.

SOLUTION

We know that iron is a bcc metal and hence it has two atoms per unit cell. Also we know its atomic weight $AW = 55.845 g \cdot mol^{-1}$ and the cell parameter $c = 286\text{pm}$. Using the metallic density formula:

$$d = \frac{2 \cdot 55.845}{286^3 \cdot 6.023 \times 10^{-7}} = \frac{111.69}{14.09} = 7.93 g \cdot ml^{-1}$$

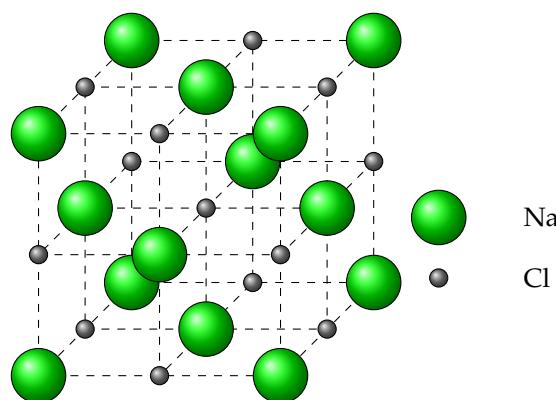
◆ STUDY CHECK

Calculate density of gold ($AW=196.96 g \cdot mol^{-1}$) knowing this is a fcc metal with cell parameter is 406pm.

Ionic solids Ionic solids have high melting point and they are typically hard. They also do not conduct the electricity in solid form. An example of an ionic solid is NaCl. The structure of NaCl and many other ionic solids results from the superposition of two different compact lattices—this is the reason these are called binary solids as they are made of two units—and each lattice is superimposed. Normally, the largest ion (Na^+) forms a packed arrangement such as fcc or ccp, and the smallest ion (Cl^-) resides on the holes of the lattice. Here we will care about constructing the formula of the unit cell, such as NaCl by counting the atoms in the unit cell.

Sample Problem 114

Calculate the formula for the following unit cell

**SOLUTION**

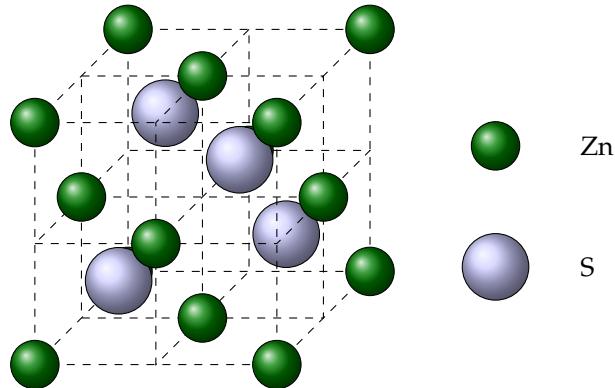
The unit cell contains Cl^- and Na^+ . Remember every location in the unit cell has different sharing factor. We will compute the number of atoms in each location and multiply by the sharing factor to calculate the number of Cl and Na in the cell:

Location	Sharing Factor, f	# atoms, N	$f \times N$
Corner	$1/8$	8Na^+	1
Faces	$1/2$	6Na^+	3
sides	$1/4$	12Cl^-	3
Inside	1	1Cl^-	1

Overall, we have Na_4Cl_4 which corresponds with the formula NaCl .

◆ STUDY CHECK

Calculate the formula for the following unit cell:



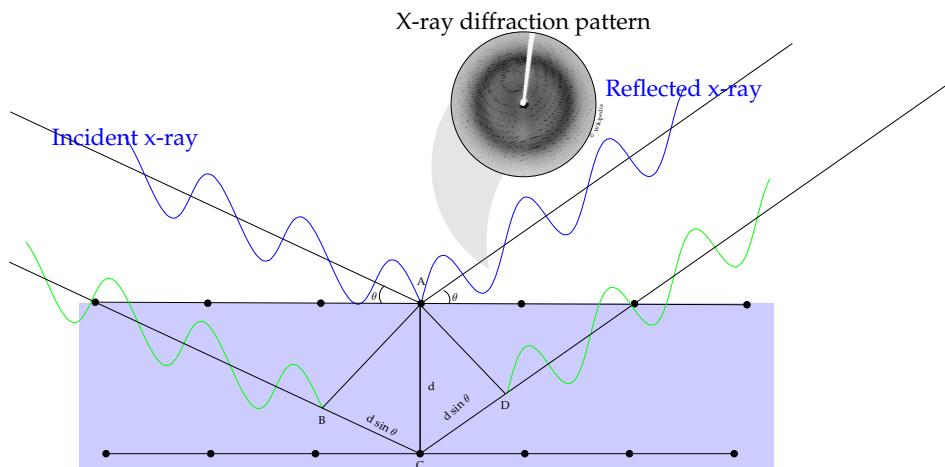


Figure 10.6 Reflection of x-rays in two different lattice points separated by a distance. The incident waves are in phase—maximums and minimums overlap—but the reflected waves are only in phase when the difference of distances traveled by both is an integral number of wavelengths. In the image $BC + CD = 2dsin\theta$.

X-ray diffraction: a method to measure cell parameters

X-ray diffraction is an experimental technique used to study the structure of solids and specifically to obtain cell parameters—the length of the unit cell that defines the structure of a crystal. X-rays, high-frequency radiation, scatter when they encounter a regular array of atoms in which the spacing is compatible with the x-ray wavelength. Diffraction results in two different types of wave interference: constructive and destructive. Constructive interference results in bright spots and destructive interference results in dark spots. Waves impacting atoms at a different lattice positions travel different distances. If the difference in distance equals to an integral number of wavelength there both rays will interfere constructively. Bragg's equation relate the cell parameter (d) of a solid with the angle (θ) of the diffracted x-rays and its wavelength (λ). The number n is called the diffraction order and represents an integer values ($n=0, 1, 2, \dots$).

$$n\lambda = 2dsin\theta \quad (10.1)$$

Sample Problem 115

We study the structure of a crystal using x-rays of 9nm, finding a first-order reflection at 20° . Calculate the distance between the planes responsible for this reflection.

SOLUTION

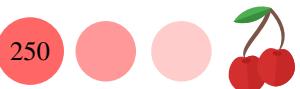
We should use Bragg's equation, using $\theta=20^\circ$, $\lambda=9\text{nm}$ and $n=1$. Solving for d we have:

$$1 \cdot 9 = 2dsin(20)$$

The calculated plane spacing is 26.3nm.

◆ STUDY CHECK

Two lattice planes separated by a distance of 4nm produce a first-order x-ray diffraction at 15° using radiation of wavelength of 3.2nm. Calculate the angle for the second-order diffraction.



▼A paper clip standing on water



© wikipedia

▼Water droplets



© www.picklist.com

▼Meniscus of water and mercury



© Flickr

▼A viscous liquid



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▼Capillary for tubes of different diameters



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This section will cover some of the properties of the liquid state. In particular the importance of the vapor pressure, the viscosity and the surface tension. All these properties are determined by the intermolecular forces that connect the molecules of a liquid.

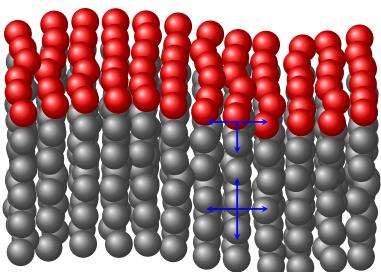
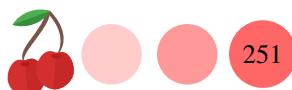


Figure 10.7 A representation of surface (red spheres) and bulk (blue spheres) liquid molecules as well as two types of meniscus: a concave and a convex meniscus, typical of water and mercury respectively. Surface molecules are pulled inwards creating the surface tension whereas bulk molecules are not.

Surface tension In a liquid there are two types of molecules, based on their location. Some molecules are located in the interior part of the liquid, far away from its surface. We call this the bulk of the liquid. Others are located at the surface of the liquid. The molecules at the bulk are surrounded by other molecules in all directions, being pushed and pulled in all directions by intermolecular forces. For these molecules, overall there is no net pull in any direction. Differently, surface molecules because of their location are surrounded by fewer molecules located on the bottom part of the surface. As such, they are pushed and pulled down and to the side by the surrounding molecules, but not upwards. As a result of this imbalance, surface molecules experience elastic forces that cause the surface of the liquid to tighten up so that the surface minimizes its surface area. The surface tension of a liquid (γ_t) is a measure of these elastic forces in the surface of the liquid. It is defined as the amount of energy needed to modify the surface of a liquid by the unit of area, with units of milli Newton per meter, mN/m. Surface tension values depend on the temperature and the phases in contact. For example, let us consider three different phases: water (a liquid), air (a gas), and mercury (a liquid). The surface tension of water in the water-air interface is different than the value for the water-mercury interface as the chemicals in contact with water are different. The stronger the intermolecular forces connecting the molecules of a given phase, the higher the surface energy—it would take more energy to modify, expand or contract, the surface of the liquid. For example, the surface tension of the H₂O-air interface (73mN/m) is stronger than the one for the C₆H₆-air interface (29mN/m), as water molecules interact by means of strong hydrogen bonds whereas the only intermolecular forces existing among the C₆H₆ are weak dispersion forces. The surface tension is responsible for phenomena such as capillary, the beading of water on the plant's leaves—water form beads or drops on the top of leaves—or the formation of the meniscus, a curved surface of a liquid in a narrow tube. In particular, capillary results from the competitive effect of cohesive and adhesive forces. In the case of mercury, the cohesive forces are stronger than the adhesive. Hence, the meniscus created is convex. In the case of water, the adhesive forces are stronger, and therefore this liquid forms a concave meniscus.



▼ Rubbing alcohol has low heat of vaporization



© wikipedia

Table 10.4 Surface tension (γ_t) values for several interfaces at different temperatures.

Interface	γ_t (mN/m)	T	Interface	γ_t (mN/m)	T
H ₂ O-Air	73	20°C	H ₂ O-Hg	415	20°C
CH ₃ I-Air	67	20°C	H ₂ O-Air	73	22°C
C ₆ H ₆ -Air	30	20°C	H ₂ O-Air	72	25°C
CH ₃ OH-Air	22	20°C	Hg-Air	486	20°C

Viscosity Viscosity (η) is the measure of a fluid's resistance to flow. High viscosity liquids flow slowly and this effect results from the intermolecular forces. Liquids with strong intermolecular forces tends to present high viscosities. Viscosity, as well as surface tension, depends on temperature and high temperature reduce the viscosity. Molecular complexity also affect viscosity and long molecules made of carbon and hydrogen have higher viscosities than small molecules due to the fact that because of their size they present more intermolecular interactions. The units of viscosity are milli Pascal-second, mPa·s.

Table 10.5 Viscosities (η) for several substances at different temperatures.

Substance	η (mPa·s)	T	Substance	η (mPa·s)	T
Benzene	0.604	25°C	Honey	5000-20000	20°C
Water	1.0016	20°C	Pitch	2.3×10^{11}	10-30°C
Mercury	1.526	25°C			
Whole milk	2.12	20°C			
Olive oil	56.2	26°C			

Vapor pressure of a liquid The molecules of a liquid in contact with the atmosphere are more likely to escape into the gas phase forming what we call the vapor pressure of the liquid. When we put a liquid in a closed container, some of the liquid molecules would go into the gas. This process is called vaporization. Whereas molecules of the gas would also go back to the liquid phase. This process is called condensation. Therefore, vaporization and condensation compete until both processes occur at the same speed and the system reaches what we call as equilibrium. The vapor pressure at this state is called the equilibrium vapor pressure or simply the vapor pressure of the liquid. This effect is responsible for the humidity the air and the smell of liquid chemicals. Chemicals with high vapor pressure vaporize readily and if they have a smell, one would be able to smell them. Solids also have vapor pressure—solids also have a smell—as their molecules are also able to escape into a gas phase.

Table 10.6 Vapor pressure (P^{vap}) for several substances at different temperatures.

Substance	P ^{vap} (mmHg)	T	Substance	P ^{vap} (mmHg)	T
Tungsten	0.75	3203°C	Carbon dioxide	42753	20°C
Ethylene glycol	3.75	20°C	Nitrous oxide	42453	25°C
Water	17.5	20°C	Carbonyl sulfide	9412	25°C
Propanol	18.0	20°C	Propane	7584	27°C
Ethanol	43.7	20°C	Formaldehyde	3268	20°C
Acetaldehyde	740	20°C	Butane	1650	20°C

▼ Acetone has low heat of vaporization



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▼ Perfumes have low vaporization heat



© Wikipedia

▼ Metals have high vaporization heat



© Wikipedia



Enthalpy of vaporization The enthalpy of vaporization of a liquid (ΔH_{vap}) is the energy needed to vaporize a liquid. This energy is often called heat of vaporization or molar heat of vaporization. Mind that ΔH_{vap} values are normally positive. This corresponds to the fact that we have to give energy to the liquid in order to create a vapor, and hence the process is endothermic. In general compounds with small heat of vaporization can vaporize easily. Think about the smell of a perfume you like. Now, think about the smell of water. Why a perfume smells and water does not. The enthalpy of vaporization of a perfume is small whereas ΔH_{vap} for water is larger (41kJ/mol). This means it is easier for the perfume molecules to escape into the gas phase and hence produce a smell. Another example is acetone–nail polish remover. This chemical has a very distinctive smell. ΔH_{vap} for acetone is 31kJ/mol. If you compare this value with the value of water you can see acetone is more likely to have a smell.

Table 10.7 Enthalpy of vaporization (ΔH_{vap}) for several substances and boiling points.

Substance	T	ΔH_{vap} (J/mol)	Substance	T	ΔH_{vap} (J/mol)
Acetone	56°C	31300	Water	100°C	40660
Aluminium	2519°C	294000	Phosphine	-88°C	14600
Ammonia	-33°C	23350	Propane	-42°C	15700
Butane	-1°C	21000	Methanol	64.7°C	35200
Ethanol	78 °C	38600	Isopropyl alcohol	83°C	44000
Hydrogen	-253°C	899.2	Iron	2862°C	340000

Sample Problem 116

Order the following compounds from high to low vapor pressure: C₆H₆ ($\Delta H_{vap}=31\text{kJ/mol}$), C₆H₅OH ($\Delta H_{vap}=39\text{kJ/mol}$), H₂O ($\Delta H_{vap}=41\text{kJ/mol}$)

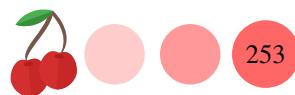
SOLUTION

The larger ΔH_{vap} the harder it is to vaporize a liquid and hence the lower the vapor pressure of the liquid. If we compare the liquids in this example, water has the lowest vapor pressure, whereas cyclohexane (C₆H₆) has the highest vapor pressure.

❖ STUDY CHECK

Order the following compounds from high to low vapor pressure (P^{vap}): NH₃ ($\Delta H_{vap}=23\text{kJ/mol}$), CH₄ ($\Delta H_{vap}=8\text{kJ/mol}$), C₄H₁₀ ($\Delta H_{vap}=15\text{kJ/mol}$)

Vapor pressure change with temperature This vapor pressure strongly depends on temperature. That is the reason why summer days can also be humid days if you live near the seaside. In particular, this change depends on the value of the heat of vaporization. The reason for this, is because at higher temperature more molecules have enough kinetic energy to escape from the liquid into the gas phase. For chemicals with low heat of vaporization we can expect a more sharp change of the vapor pressure with temperature. The following formula gives the relation between vapor pressure and temperature. Mind that for every temperature we will have a



vapor pressure value. In the formula you will need two pairs of temperatures and hence two pairs of vapor pressures:

$$\ln\left(\frac{P_{T_1}^{vap}}{P_{T_2}^{vap}}\right) = \frac{\Delta H_{vap}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Clausius-Clapeyron relation

where:

$P_{T_1}^{vap}$ is the vapor pressure at temperature T_1 in Kelvin

$P_{T_2}^{vap}$ is the vapor pressure at temperature T_2 in Kelvin

ΔH_{vap} is the enthalpy of vaporization in $J \cdot mol^{-1}$

$R=8.314 J \cdot K^{-1} mol^{-1}$ is the constant of the gases in energy units

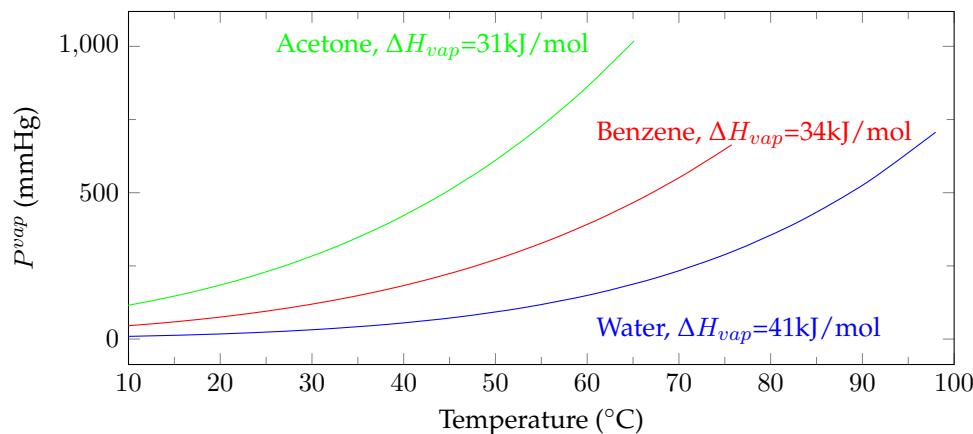


Figure 10.8 Vapor pressure change with temperature for three chemicals with different heat of vaporization.

Sample Problem 117

The vapor pressure of water at 298K is 0.03 atm. Calculate the vapor pressure of water at 323K given $\Delta H_{vap} = 43.9 KJ \cdot mol^{-1}$.

SOLUTION

In order to use the Clausius-Clapeyron relation we need two pairs of (T , P^{vap}) values. In this problem, we have the value of the vapor pressure at 298K, hence we have (298K, 0.03 atm) and they ask the pressure at 323K. Therefore the second pair is (298K, x atm), where X is the vapor pressure at 298—what they are asking in the problem. We can call (298K, 0.03 atm) as $(T_1, P_{T_1}^{vap})$ and (298K, X atm) as $(T_2, P_{T_2}^{vap})$. At this point we have $T_1 = 298K$ and $P_{T_1}^{vap} = 0.03 \text{ atm}$ and $T_2 = 323K$ and $P_{T_2}^{vap} = x$. We also have the enthalpy of vaporization. Note that this value has to be given in $J \cdot mol^{-1}$ and hence, we will use $\Delta H_{vap} = 43.9 \times 10^3 J \cdot mol^{-1}$. Now we can plug these values into the formula:

$$\ln\left(\frac{0.03}{x}\right) = \frac{43.9 \times 10^3}{8.314} \left(\frac{1}{323} - \frac{1}{298}\right)$$



Let us solve this step by step. First we solve the part on the right:

$$\ln\left(\frac{0.03}{x}\right) = -1.37$$

Now, in order to eliminate the logarithm we should use the exponential function in both sides:

$$\frac{0.03}{x} = e^{-1.37}$$

Calculating the exponential of -1.37 we have:

$$\frac{0.03}{x} = 0.25$$

That leads to a x value of 0.12 atm.

◆ STUDY CHECK

Using the data below, calculate ΔH_{vap} for HNO_3 .

T (K)	P^{vap} (mmHg)
10	26.6
20	47.9
30	81.3

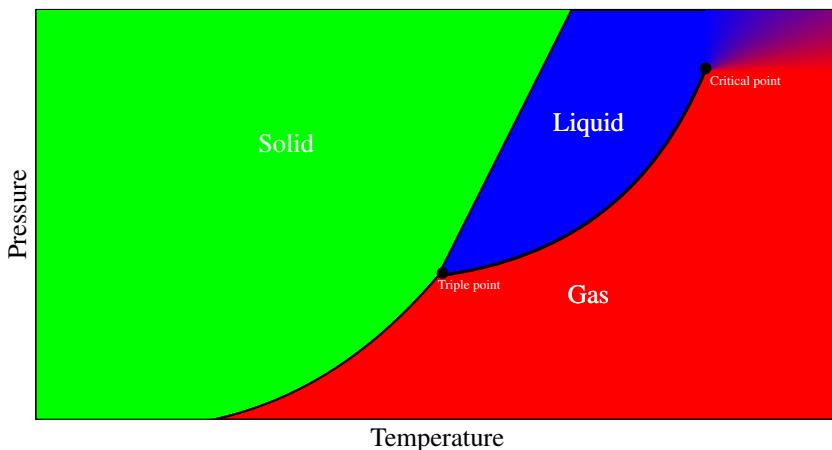
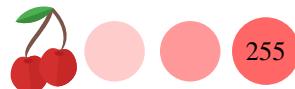


Figure 10.9 A typical phase diagram showing the different phases, the critical and the triple point. As the slope of the line that separates liquid and gas has an angle lower than 90° the solid phase has higher density than the liquid.

10.5 Phase diagrams

Water can be found at different states: liquid, solid and gas. We know at room temperature—and atmospheric pressure—water is a liquid. However, what if we warm up a sample of water? When does it become vapor? And more importantly, what if the working pressure is not one atmosphere? Would water boil the same near the sea or on top of a mountain? The answer to all these questions can be found in the phase diagram of water. This section



will cover phase diagrams. You will learn how to read phase diagrams in order to predict the state of matter at any temperature and pressure conditions. You will also learn how to identify critical and triple points.

Description of a phase diagram: important points A phase diagram is a representation of the different temperature and pressure conditions in which we can find the different states of matter of a substance. Normally, temperature is listed in the horizontal axis and pressure in the vertical axis. The different phase, liquid, solid and gas, are listed. At low temperature we tend to find solids and gases are common at high temperature. Similarly, at low pressures we tend to find gases and solids at high pressure. With pressure we refer to compressive pressure. The lines in a phase diagram represent equilibrium and the line separating solid and gas represents all the pressure and temperature conditions in which we can find a gas in equilibrium with a liquid. Similarly, the line separating liquid and solid represents all the pressure and temperature conditions in which we can find a liquid in equilibrium with a solid. With equilibrium, we mean that both phase are present and the process of phase transition proceeds at the same speed in both directions. There are two important points in a phase diagram: the critical point and the triple point. The triple point is the pressure and temperature conditions in which the three phases—solid, liquid and gas—coexist. Another important point is the critical point. Beyond this point one cannot liquefy (go from gas into a liquid) or condense (go from liquid into a gas) the substance. There is one more important feature one can extract from a phase diagram. Normally, but not always, solids are more dense than liquids. We can compare the density of the solid and the liquid by analyzing the slope of the line connecting both phase. If the slope is lower than 90° then the solid will be more dense than the liquid. If it is larger than 90° then the solid is less dense than the liquid. If the slope is 90° then both liquid and solid have the same density.

What are normal conditions? When we speak about normal conditions we refer to a pressure of 1atm, which is the common atmospheric pressure. But remember that the atmospheric pressure depends on the height of the location where measured. And locations near the sea—at low height—tend to have higher pressure than locations near the mountains—at a larger height.

Phase transition terminology Each phase transition has a specific name. You may be familiar with some of the terms like freezing that involves the change from liquid to solid. Other names are listed below:

Liquid \longrightarrow Solid

Freezing

Liquid \longrightarrow Gas

Evaporation or vaporization

Solid \longrightarrow Liquid

Melting

Gas \longrightarrow Liquid

Condensation

Solid \longrightarrow Gas

Sublimation

Gas or Solid \longrightarrow Liquid

Liquefy

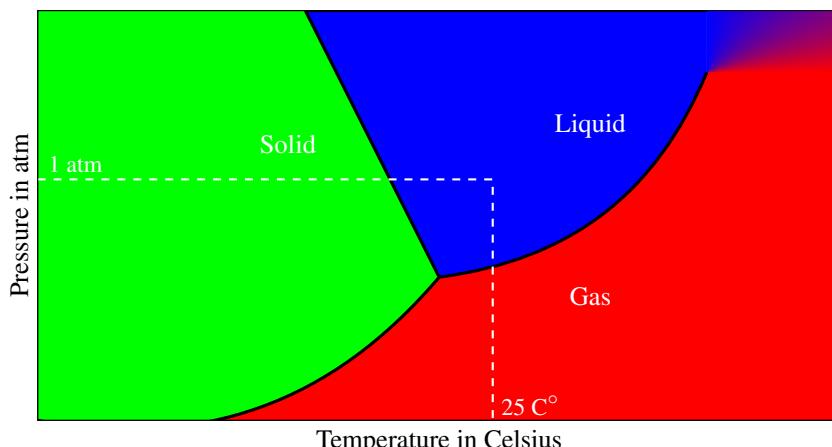


Figure 10.10 The phase diagram of water with pressure in the Y axis and temperature in the X axis. This diagram displays the different states of matter of water for different pressure and temperature conditions. The coordinates of the triple point are ($0.0098\text{ C}^{\circ}, 0.0060\text{ atm}$). This means that at this low pressure and temperature conditions we have three phases in contact: water, ice and steam. The coordinates of the critical point are ($374\text{ C}^{\circ}, 218\text{ atm}$). This means that for temperature beyond 374 C° it is not possible to liquefy steam.

Phase diagram of water A phase diagram is just a diagram with temperature in the X axis and pressure in the Y axis. It tells you whether you have gas, liquid or gas at a large range of pressure and temperature conditions. For example, the figure on the side of the page presents the phase diagram of water and the line indicates the phase present at (Temperature, Pressure) conditions of ($25\text{ C}^{\circ}, 1\text{ atm}$). Obviously, this phase is liquid water. *Normal conditions* refer to pressure conditions of 1 atm. Hence, we say that the normal boiling point of water—this means at 1 atm—is 100 C° . In the following we will analyze a set of experiments represented as vertical and horizontal lines in the diagram. Horizontal lines are cooling/heating experiments in which pressure is kept fixed and temperature changes. Vertical lines represent compression/decompression experiments in which pressure changes at constant temperature.

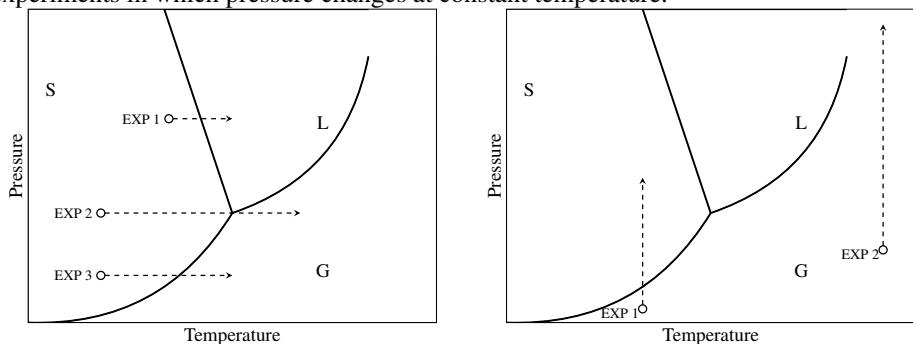
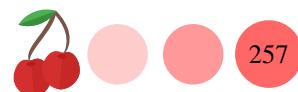


Figure 10.11 Heating experiments (left) and compression experiments (right).

Heating and compression experiments We will analyze now some cooling/heating experiments. In the first experiment, we start by having a solid that we heat up to obtain first a mixture between liquid and solid and then a pure liquid. In this experiment we just transitioned between solid into a liquid. Experiment 2 is different. We also start by having a solid. The difference is that this time we reach a point called *triple point* in this point the three phase coexist at a single pressure and temperature. Therefore, in this experiment, we go from a solid into a mixture of solid, liquid and



gas. After that we transition directly into a gas. Experiment number three is called sublimation. In this experiment we start by having a solid that transitions into a gas by means of a mixture of solid and gas. We can also discuss some compression/decompression experiments. The first experiment is a compression experiment in which we start from a gas and we end up having a liquid by means of a mixture of both. The second experiment starts beyond the *critical point* and hence even if you compress the gas you will never reach a liquid state. The critical point is the point beyond which one cannot liquefy a gas or gasify a liquid.

Energy calculations involving phase transitions The enthalpy of vaporization of a substance gives you the amount of energy needed to vaporize an amount of substance. Similarly, the enthalpy of fusion tells you about the energy involved in the fusion process. Each phase—gas, liquid and vapor—has different specific heat. Using water as an example, imagine we need to calculate the energy involved in the heating of $m=18\text{ grams}$ ($n=1\text{ mole}$) of water from 20°C to a 150°C . This energy results from three contributions: the energy needed to warm up liquid from 20°C to a 100°C (we can call this ΔT_1), the energy to boil 1 mole of water, and the energy to warm up 1 mole of gas water from 100°C to a 150°C (we can call this ΔT_2). The final calculation will be:

$$Q = m \cdot c_e^{\text{H}_2\text{O}(\ell)} \cdot \Delta T_1 + n \cdot \Delta H_{vap}^{\text{H}_2\text{O}} + m \cdot c_e^{\text{H}_2\text{O(g)}} \cdot \Delta T_2$$

Table 10.8 Properties of the different states of matter of water.

Property	Ice	Water	Steam
Density (g/mL)	0.93	1	0.6
$c_e (\text{J}\cdot\text{g}^{-1}\cdot{}^\circ\text{C}^{-1})$	2.18	4.184	1.99
ΔH_{fusion} (kJ/mol)	6.01		
ΔH_{vap} (kJ/mol)		44	

**Funny facts!**

Water is weird. Everyone knows the chemical symbol for water is H_2O , and that all living things need water to survive. Here are eight facts about weird water that you might not know!

1. Water is alien. All water on earth arrived as ice on asteroids and comets from space.
2. All water on earth has been recycled through animals, plants, rocks, oceans, and clouds. In other words, you're drinking dinosaur pee.
3. Water doesn't follow the normal rules of chemistry. Water is made of two elements: oxygen and hydrogen, both of which are very light. The rules of chemistry say that on earth, liquid water should not exist. Instead, if water followed the rules, it would exist on earth only as water vapor.
4. Water is the only chemical that expands when it goes from a liquid to a solid. Because solid water, aka ice, is less dense than liquid water, ice floats. This allows ice to insulate the liquid water underneath it. Without this unique property, life would not have survived earth's many ice ages.
5. Hot water freezes faster than cold water, and no one knows why. This is known as the Mpemba effect, named after the Tanzanian student who discovered this phenomenon.
6. Water molecules are so good at sticking to each other that they can overcome the force of gravity. In biology, this is called capillary action and is the mechanism that allows plants to move water from their roots to their leaves. This unique property of water also allows oxygen and nutrients to reach the outermost edges of your brain.
7. Water is the second most common molecule in the universe, after molecular hydrogen. There's water on Mars, the moon, and almost every other object in our solar system, including Pluto.
8. Water is a universal solvent. Water is able to break most chemical bonds and dissolve most chemicals. It is very difficult to create pure water even in a laboratory setting, as nearly all chemical compounds will dissolve in water. This makes water one of the most reactive compounds known to man.



CHAPTER 10

INTERMOLECULAR FORCES

10.1 Indicate the strongest intermolecular force existing between the molecules of the following compounds:
 (a) CH₃OH (b) H₂ (c) CCl₄

10.2 Indicate the strongest intermolecular force existing between the molecules of the following compounds:
 (a) CH₄ (b) CCl₃H (c) HF (d) HCl

10.3 From the following pair of molecules, which molecule forms intermolecular H bonds? (a) HF or H₂
 (b) NH₃ or CH₄

10.4 From the following pair of molecules, which molecule forms intermolecular H bonds?
 (a) CH₃—O—CH₃ or H₂O (b) HCl or HF

10.5 From the following pair of molecules, which molecule forms stronger dispersion forces? (a) Ar or He (b) H₂O or H₂S

10.6 From the following pair of molecules, which molecule forms stronger dispersion forces? (a) CH₃CH₃ or CH₄ (b) CH₄ or CH₃Cl

10.7 From the following pair of molecules, which molecule forms stronger dipole forces? (a) HCl or HBr (b) H₂O or H₂S

10.8 From the following pair of molecules, which molecule forms stronger dipole forces? (a) NH₃ or H₂O (b) HI or HBr

10.9 From the following pair of molecules, which molecule has higher boiling point? (a) CH₃CH₃ or CH₄ (b) CO₂ or H₂O

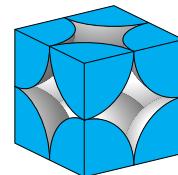
10.10 From the following pair of molecules, which molecule has higher boiling point? (a) HF or HCl (b) Ar or He

THE SOLID STATE

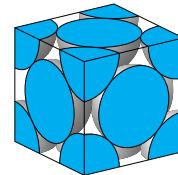
10.11 Indicate the number of atoms contained in the body-centered (bcc) cubic unit cell, for structures with the same type of atoms.

10.12 Indicate the number of atoms contained in the simple cubic (sc) unit cell, for structures with the same type of atoms?

10.13 The image displays the structure of Polonium. What is the number of atoms per unit cell for this metal?



10.14 The image displays the structure of Gold. What is the number of atoms per unit cell for this metal?

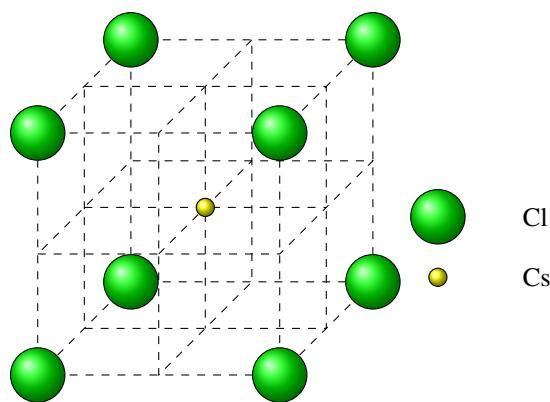


10.15 Identify the type of crystalline solid formed by the following compounds: (a) cesium chloride (b) tungsten

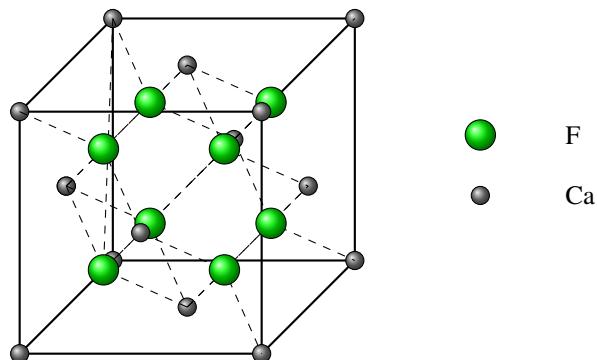
10.16 Identify the type of crystalline solid formed by the following compounds: (a) acetic acid (b) hydrogen sulfide

10.17 An element crystallizes in a face-centered cubic lattice and has a density of $1.5 \text{ g} \cdot \text{mL}^{-1}$ and a cell parameter of 452pm. Calculate the approximate mass of the element.

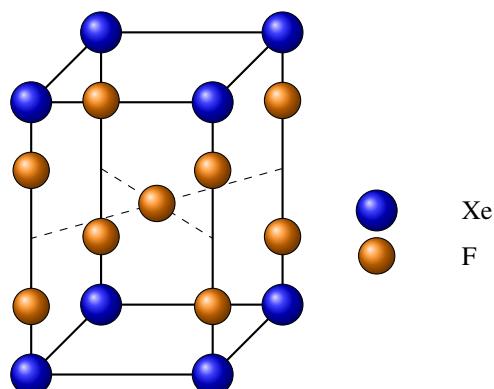
10.18 Calculate the formula for the following unit cell (the unit formula):



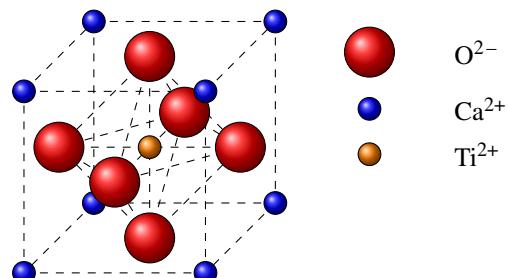
10.19 Calculate the formula for the following unit cell:



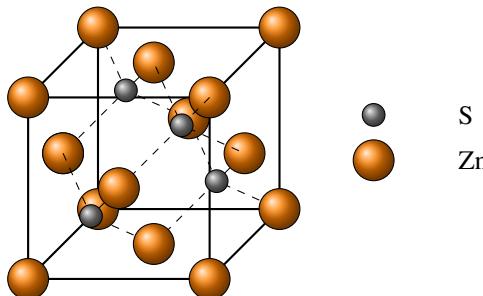
10.20 Calculate the formula for the following unit cell:



10.21 Calculate the formula for the following unit cell:

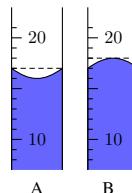


10.22 Calculate the formula for the following unit cell:

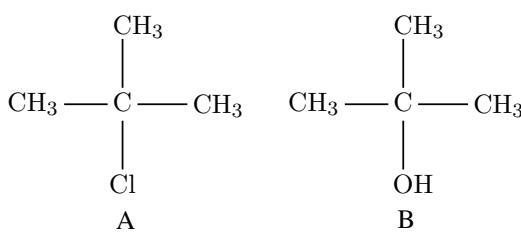


LIQUID STATE

10.23 Answer the following questions based on the image below: (a) Identify each meniscus as concave or convex (b) Which liquid has higher surface tension (c) Which liquid is more wettable (wets more)



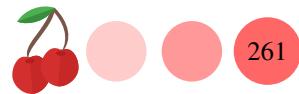
10.24 Which of the following molecules present higher viscosity?



10.25 A liquid has a enthalpy of vaporization of 30 kJ/mol and a boiling point of 122°C at 1.00 atm . Calculate its vapor pressure at 200°C .

10.26 What is the enthalpy of vaporization of a liquid that has a vapor pressure of 500 torr at 100°C and a boiling point of 90°C at 460 torr ?

10.27 The vapor pressure of a chemical at 32°C is 0.86 atm . Given that its heat of vaporization is 26 kJ/mol , calculate the vapor pressure at 50°C .



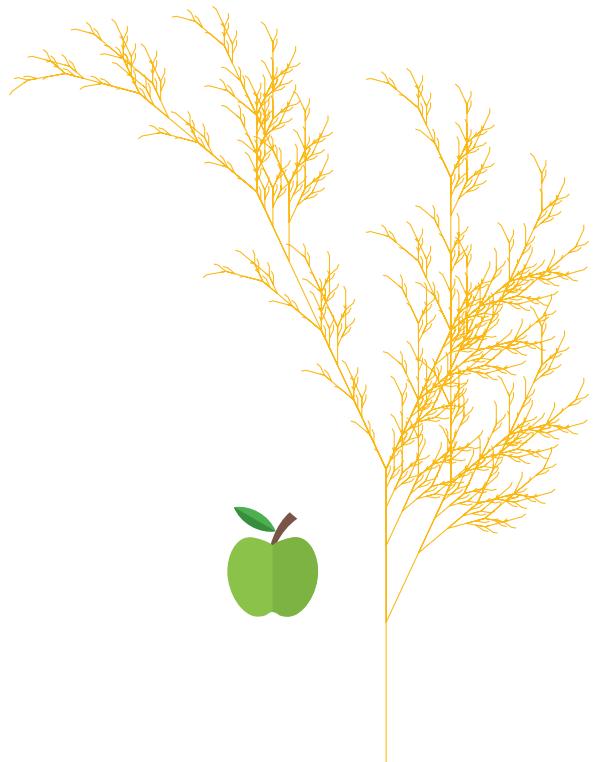
10.28 Calculate the heat of vaporization of a chemical that doubles its vapor pressure when the temperature increases from 10°C to 40°C.

10.29 At what temperature in K will the vapor pressure of a chemical with 200kJ/mol heat of vaporization be three times the value at 298K?

10.30 Given that the vapor pressure at 33°C is 63mmHg for a chemical with molar heat of vaporization of 44kJ/mol, calculate the normal boiling point of this chemical—this is the boiling point at 760mmHg.

10.31 Order the following compounds from high to low vapor pressure (P^{vap}): NH₃ ($\Delta H_{vap}=23\text{ kJ/mol}$), CH₄ ($\Delta H_{vap}=8\text{ kJ/mol}$), C₄H₁₀ ($\Delta H_{vap}=15\text{ kJ/mol}$)

10.32 Order the following compounds from high to low vapor pressure: C₆H₆ ($\Delta H_{vap}=31\text{ kJ/mol}$), C₆H₅OH ($\Delta H_{vap}=39\text{ kJ/mol}$), H₂O ($\Delta H_{vap}=41\text{ kJ/mol}$)



College Chemistry

A Comprehensive Set of Imperfect Notes

This set of lectures present content in a simple and clear way, while including numerous worked examples and many problems with solution. In particular, this current version of the manuscript contains more than 90 solved problems and more than 200 problems with solution. It also contains numerous diagrams and graphs specifically developed to clarify the content. The organization of the note intends to help the reader digest the large content typically covered in a GOB or college Chemistry class. Every part ends with a review quiz that assesses content.