



College Chemistry

A Comprehensive Set of Imperfect Notes

Daniel Torres



December 3, 2020 (V 0.2)

Periodic Table of Chemical Elements

Periodic Table of Elements																			
		Group 1		Group 2						Groups 13-18									
		H		He						Boron Period									
1	1.0079	Hydrogen	H	2 IIA		15 IIIA						14 VA	15 VA	16 VA	17 VIIA	Helium			
3	6.941	4	9.01212	Be	Beryllium	B	C	N	O	F	Ne	Fluorine	15.999	9	18.998	10	20.180		
11	22.990	12	Mg	3 IIIB	4 IVB	5 VB	6 VIIB	7 VIIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIIB	Al	Si	P	S	Cl	Ar
19	39.098	20	40.078	Ca	S	Ti	V	Cr	Mn	Fe	Co	Zn	Ga	Ge	As	Se	Br	Kr	Xe
37	85.468	38	87.62	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Te	I	Xe
55	132.91	56	137.35	Ba	La-Lu	Hf	Ta	W	Re	Os	Rhodium	Palladium	Silver	Cadmium	Indium	Antimony	Teinium	Iodine	Xenon
87	Fr	88	226	Ra	Ac-Lr	D ₄₅	D ₅₀	D ₅₅	Sq	Bh	Hs	Mt	Rg	Uut	Uuh	Uup	Uus	Uuo	Uun
		Name		Symbol						z mass						Name			
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 Alkali Metal	 Alkaline Earth Metal	 Metal	 Metalloid	 Non-metal	 Halogen	 Noble Gas	 Lanthanide/Actinide
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18 VIII A

Contents

PART A	2
1 Measurements	1
PART B	17
2 The periodic table: atoms and Elements	19
3 Chemical naming	33
PART C	52
4 The Mole and Chemical Reactions	55
PART D	75
5 Reactions in solution	77
6 Gases	97
PART E	119
7 Thermochemistry	121
8 Solids and liquids	143
PART F	168
9 Electronic structure of atoms	171
10 Electronic structure of molecules	205

TO THE READER

First and foremost, I genuinely care about the progress of each and 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. These notes start with the fundamentals and—at this point—end with solids and liquids. 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 in order to break down the very basics of the 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 in order to find the solution based on the information presented. As you study this set of lecture, I encourage you to read the different section of a chapter, highlight the main ideas and find key words that represent new concepts. Numerous examples are presented along 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 are 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 along this guide to help you focus on the most relevant content. For example, *yellow notes* are used to indicate important formulas or tables. Also, when the numerical problems get to 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 student often rely on textbooks to learn. These valuable educational resources are often used for a very limited period of time 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 for 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 lecture is indeed imperfect, and hence its title. Yet, it is the result of many hours of

work—indeed months of work. Still, it contains typos and often times incorrect answers. 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 correspond to the educators' point of view.

This set of lecture does not intent to replace any textbook. Indeed, there are many high-quality textbooks in the literature that I recommend:

- 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

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 L^AT_EX 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—helps makes chemistry more apparent to the viewer. One of the weak points of many open education chemistry guides are the visuals. They tend to be simplistic with low quality. This guide extensively relies on images and diagrams and uses Tikz and other open-source tools to generate diagrams. 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.



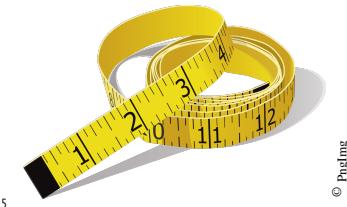
Daniel Torres
New York City

PART A

1

Measurements

M EASURING 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. This chapter will cover how to accurately measure properties and, more importantly, how to transform measurements using prefixes and unit conversions. In this chapter, by learning how to measure and perform operations with units, you will gain experience performing basic chemistry calculations.



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1.1 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 two main systems: the English System used in the US and the Metric System used by most of the industrialized world. The *Metric System* (MS) is used by scientists throughout the world and is the most common measuring system based on the meter. The *International System of Units* (SI) adopted the metric system in 1960 in order to provide additional uniformity for units used the sciences. This chapter will be mostly based on the SI units. In the following we will introduce some common units.

Length What is your height? 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: meter, inch and mile.

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GOALS

- 1 Identify units and prefixes
- 2 Introduce/eliminate prefixes
- 3 Switch prefixes
- 4 Calculate significant figures
- 5 Carry out density calculations

Discussion: (a) Discuss why is chemistry important for your career objective by listing three reasons that links chemistry with your career objective, (b) You have a glass filled with water and ice to its rim. If the ice melts will the water overflow the glass? Explain your reasoning.

Volume How much milk do you usually buy? Maybe a gallon. Volume is the amount of space that a substance occupies. A liter (L) 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 every-day 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.

Mass What is you 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 than with mass. However, mass and weight are not exactly the same, as weight is a measure of the gravitational pull on an object. It differs depending on your location in the earth—in particular the

▼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



© Pixabay

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



© www.weberscientific.com

height of your location. In the metric system, the unit for mass is the gram (g). The SI unit of mass, the kilogram (kg), is used for larger masses such as body weight. 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 ($^{\circ}\text{C}$), Fahrenheit ($^{\circ}\text{F}$), or kelvins (K).

Time How long is your commute to from home 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.

Sample Problem 1

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

- (a) 1foot (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) 800F (b) 1m³ (c) 3m (d) 67s

Answer: (a) temperature; (b) volume; (c) length; (d) time;

Table 1.1 Different unit systems

Measurements	Metric System	International System (SI)	English System
Length	Meter (m)	Meter (m)	Foot (f)
Volume	Liter (L)	Cubic meter (m^3)	Gallon (gal)
Mass	Gram (g)	Kilogram (kg)	Pound (lb)
Time	Second (s)	Second (s)	Second (s)
Temperature	Celsius ($^{\circ}\text{C}$)	Kelvin (K)	Fahrenheit ($^{\circ}\text{F}$)

1.2 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. Kilometer is larger than meter, whereas centimeter is smaller than a meter. Prefixes such as kilo or centi are attached to units in order 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. Table 1.1 lists some of the metric prefixes, their symbols, and their decimal values.

Table 1.2 Different prefixes

Prefix	Symbol	Meaning	Value
peta	P	1000000000000000	1×10^{15}
tera	T	100000000000	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	0.00000000001	1×10^{-12}
femto	f	0.000000000000001	1×10^{-15}

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 which refers to length. Another example, 7 kg means kilogram. 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.

65

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

70

How to write unit equalities and conversion factors Unit

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

Remember: the **prefix** always comes first as the **c** in **cm**

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

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

75

Remember: **equalities** are written in line whereas **conversion factors** with a fraction.

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

Sample Problem 2

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) $\frac{\underline{\hspace{2cm}}\text{s}}{1\text{Ms}}$

Answer: (a) $1\text{cs} = 1 \times 10^{-2}\text{s}$; (b) $\frac{1 \times 10^{12}\text{s}}{1\text{Ts}}$; (c) $\frac{1 \times 10^6\text{s}}{1\text{Ms}}$;

80

1.3 Using Conversion Factors

Unit equalities in the form of conversion factors are used to convert a 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 example.

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) in 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 placing the prefix at the bottom of the fraction. This will cancel out the prefix in the original unit and in the bottom part of the conversion factor, hence leaving the final unit on top of the conversion factor. The arrangement would be:

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

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:

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

Sample Problem 3

The length of a textbook page is 20cm. Convert 20cm to m.

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 $\frac{1 \times 10^{-2}m}{1cm}$:

$$20\text{cm} \times \frac{1 \times 10^{-2}m}{1cm} = 0.2m$$

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.

$$\text{Answer: } 100\text{m} \times \frac{km}{1 \times 10^3\text{m}} = 0.1\text{km.}$$

Switching prefixes In order 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:

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

Sample Problem 4

The length of a textbook page is 20cm. How many mm correspond this length.

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: $\frac{1 \times 10^{-2}m}{1cm}$ and $\frac{1 \times 10^{-3}m}{1mm}$. You will have to arrange the number (20cm) and the two conversion factors in the following form:

$$20\text{cm} \times \frac{1 \times 10^{-2}\text{m}}{1\text{cm}} \times \frac{1\text{mm}}{1 \times 10^{-3}\text{m}} = 200\text{mm}$$

◆ STUDY CHECK

Convert 100mm to km.

$$\text{Answer: } 100\text{mm} \times \frac{1 \times 10^{-3}\text{m}}{1\text{mm}} \times \frac{1\text{km}}{1 \times 10^3\text{m}} = 1 \times 10^{-4}\text{km.}$$

Square or cubic units How big is your apartment? You might be living in a 750ft^2 loft in Brooklyn or in a larger house Upstate. Often times we encounter cubic or square units such as cubic centimeter (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 $1\text{cm}^2 = 1 \times (10^{-2})^2\text{m}^2 = 1 \times 10^{-4}\text{m}^2$.

☞ Remember: the number 1×10^{-3} is **scientific notation** and must be typed in the calculator as: 1×-3 .

☞ Remember: if you use a power on a power of ten, the power and the ten exponent multiplies, and for example $1 \times (10^{-2})^2$ is 1×10^{-4} or $1 \times (10^{-4})^3$ is 1×10^{-12} .

Also the power key in your calculator is 

Another example, for the case of mm and mm^3 :

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

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

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

Sample Problem 5

How many m^2 is $20cm^2$.

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 : $\frac{1 \times 10^{-4}m^2}{1cm^2}$ or $\frac{1cm^2}{1 \times 10^{-4}m^2}$.

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

◆ STUDY CHECK

Convert $100m^3$ to dm^3 .

$$\text{Answer: } 100m^3 \times \frac{1dm^3}{1 \times 10^{-3}m^3} = 1 \times 10^5 dm^3.$$

90

Units of volume 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. In fact one liter is the same as one dm^3 and one mL is the same as one cm^3 . In the allied health field, the units mL is also written as cc as in cubic centiliters.

$$1L = 1dm^3 \quad \text{and} \quad 1mL = 1cm^3$$

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

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

Sample Problem 6

Convert $30 m^3$ into L.

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.

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

◆ STUDY CHECK

Convert 40L to cm^3 .

$$\text{Answer: } 40L \times \frac{1mL}{1 \times 10^{-3}L} \times \frac{1cm^3}{1mL} = 4 \times 10^4 cm^3.$$

Using other equalities How many hours is 300 minutes, or how many centimeters is 2 inches? Some of the units conversion are not based on a power of ten relationship such as the ones in Table 1.2. Table 1.3 lists some of the common equalities that can be easily converted into conversion factor. 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 $\frac{1\text{h}}{60\text{min}}$.

95

Table 1.3 Table containing some common unit equalities

Unit	Equality
Inches (in)-centimeters (cm)	$2.54\text{ cm} = 1\text{ in}$
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)	$1\text{ mL} = 15\text{ drops}$

Sample Problem 7

Convert 20 in to cm.

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:

$$20\cancel{\text{in}} \times \frac{2.54\text{cm}}{1\cancel{\text{in}}} = 50.80\text{cm}$$

◆ **STUDY CHECK** Convert 200mL to drops.

$$\text{Answer: } 200\cancel{\text{mL}} \times \frac{15\text{drops}}{1\cancel{\text{mL}}} = 3000\text{drops} = 3 \times 10^3\text{drops}$$

100

1.4 Significant Figures

Exact numbers results from counting. For example, think about how many eggs are there in your refrigerator, there might be three and this number is an exact number. Differently, numbers that results from a measurement are called measured values and they are subject to uncertainty—in another words error. For example, if you weight a single egg in an scale depending of the type of scale you used 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, 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 calculation in order to express the result with the right number of digits and significant figures.

105

110

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 neither the first nor the second rule. A final example,

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

¶ **Exception 3** A zero in a number expressed on 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 8

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 three 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.

Answer: 4560 has 3SF, 0.123 has 3SF, 1000 has 1SF and 0.0030 has 2SF.

Significant figures in calculations There are two different rules that allow you to express the result of a calculation 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:
120

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

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:
125

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

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:
130

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

Sample Problem 9

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: $(24.56 + 2.433) \times 0.013$

Answer: 0.35

1.5 Matter and density

We can classify chemical substances in terms of what they are made of. Some are made of just one thing, others contain different components. At the same time, some substances look like they are made of one thing and indeed they are made of many components. This section covers the classification of matter according to the purity of substances and mixtures. It also elaborates on the types of mixtures one can find. The final part of the section deals with density.

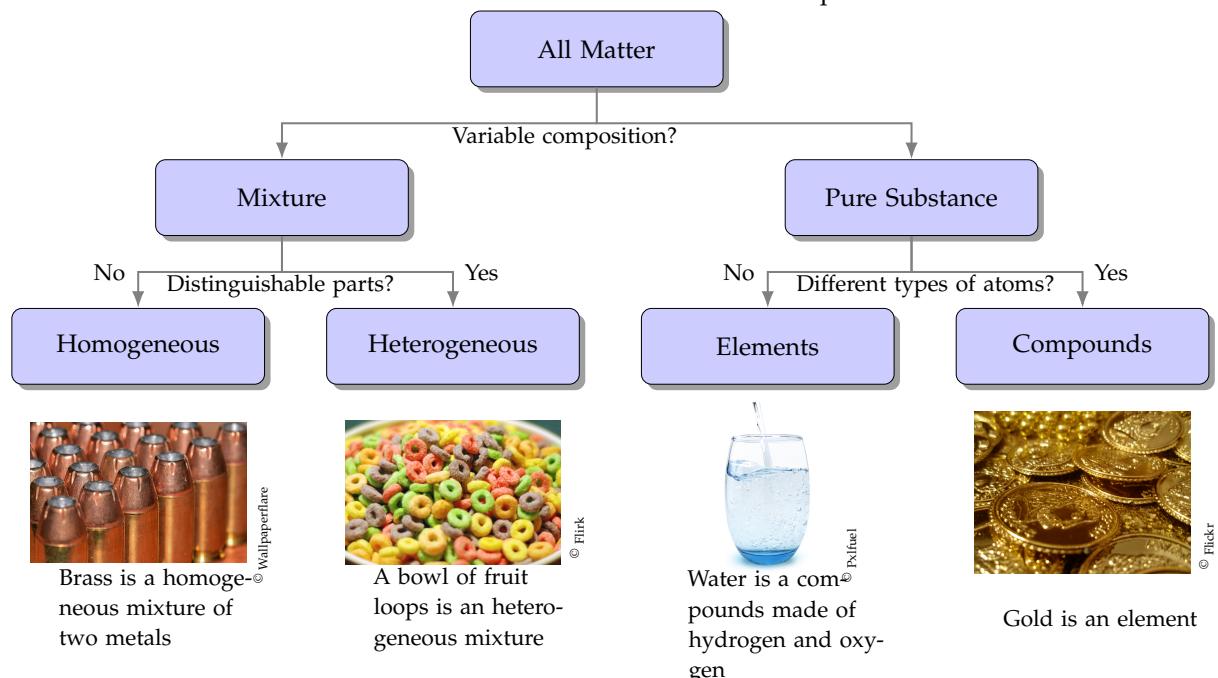


Figure 1.1 Classification of the matter

140 Pure Substances and mixtures Pure substances have a definite composition, that is, are only made of one thing. There are two different types of pure substances: elements and compounds. *Elements* are composed of only one type of atom. Examples are silver, iron, and aluminum that all contain one type of substance, and iron is only made of iron atoms, for example. *Compounds* are combinations of different elements. For example, water, H_2O is made of a combination of hydrogen and oxygen atoms. *Mixtures* are physical combinations of different substances. For example, air is a mixture of oxygen and nitrogen.

Types of Mixture Mixtures can be homogeneous or heterogeneous. In a *homogeneous mixture*—also known as solutions—the composition is uniform throughout the sample. An example of an homogeneous mixture is air, which contains oxygen and nitrogen or 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.

Sample Problem 10

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

Answer: (a) homog. mix.; (b) compound; (c) element; (d) heterog. mix.

Density Density refers to the mass of a substance with respect to its volume.

This is an unique property for each substance. 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.
160

The formula for density is

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

Density and mixing A small piece of ice will float on water. The reason for that is density: density of ice (0.9g/mL) is smaller than density of water (1.0g/mL) and hence ice will stay on top of water. Objects with density larger than 1 g/mL will sink whereas objects with density smaller than this value 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 .
165

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 $T < 273.15 \text{ K}$

Sample Problem 11

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.

Volume by displacement We can use density to calculate the volume of an unknown solid without having to physically measure the dimensions of the object. We will explain how to do this in the following example.

Sample Problem 12

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

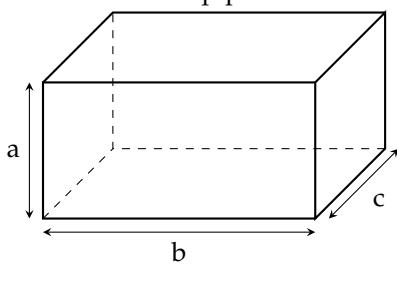
A lead weight used in the belt of a scuba diver has a mass of 226 g. When the weight is placed in a graduated cylinder containing 200.0 mL of water, the water level rises to 220.0 mL. What is the density of the lead weight (g/mL)?

Answer: 11.3 g/mL.

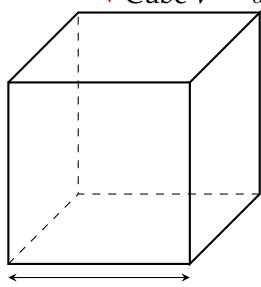
175

Density and the volume of objects Density depends on volume and in particular the larger volume the smaller density. In the Figure below you can find formulas to calculate the volume of some common objects like an sphere or a cube.

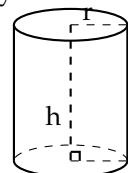
▼ Parallelepiped $V = abc$



▼ Cube $V = a^3$



▼ Cylinder $V = \pi r^2 h$



▼ Sphere $V = \frac{4}{3}\pi r^3$

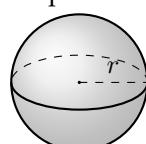


Figure 1.2 Volume of some objects

180

CHAPTER 1

UNITS AND MEASUREMENTS

1.1 Solve for x in the following algebraic equations:

(a) $3x + 1 = 5$

(d) $\frac{3x+1}{2} = 2$

(b) $2x - 1 = 5$

(e) $\frac{2x-1}{3} = 2$

(c) $\frac{3}{2} = \frac{1}{2x}$

(f) $\frac{2}{3} = \frac{1}{3x}$

1.2 Compute the following calculations involving scientific notation:

(a) $\frac{6.5 \times 10^3}{3 \times 10^2}$

(c) $\frac{1.3 \times 10^{-3}}{2.5 \times 10^{-2}}$

(b) $\frac{6.1 \times 10^{-3}}{3 \times 10^4}$

(d) $\frac{2.4 \times 10^{-3}}{5.4 \times 10^{-6}}$

1.3 Indicate the magnitude measure in the following measurements: (a) 2 L (b) 5 cm

1.4 Answer the following questions: (a) Indicate the metric base unit for mass (b) Indicate the metric base unit for mass (c) Indicate metric base unit for volume (d) Indicate basic unit of mass in the SI (e) What magnitude measures the amount of space occupied by a substance

PREFIXES & CONVERSION FACTORS

1.5 Fill the gap in the following unit equalities or conversion factors: $1dm = \underline{\hspace{2cm}} m$

1.6 Fill the gap in the following unit equalities or conversion factors: $1cm = \underline{\hspace{2cm}} m$

1.7 Fill the gap in the following unit equalities or conversion factors: $\frac{1nm}{\underline{\hspace{2cm}} m}$

1.8 Fill the gap in the following unit equalities or conversion factors: $\frac{1fs}{\underline{\hspace{2cm}} s}$

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

$1Tm = \underline{\hspace{2cm}} m$

$1qt = \underline{\hspace{2cm}} mL$

$1dm = \underline{\hspace{2cm}} m$

$1L = \underline{\hspace{2cm}} dm^3$

$1cg = \underline{\hspace{2cm}} g$

$1lb = \underline{\hspace{2cm}} g$

$1ms = \underline{\hspace{2cm}} s$

$1in = \underline{\hspace{2cm}} cm$

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

(a) $\frac{1km}{\underline{\hspace{2cm}} m}$

(d) $\frac{\underline{\hspace{2cm}} L}{10^{-3}L}$

(b) $\frac{1cm}{\underline{\hspace{2cm}} m}$

(e) $\frac{\underline{\hspace{2cm}} L}{10^{-2}L}$

(c) $\frac{1ms}{\underline{\hspace{2cm}} s}$

(f) $\frac{\underline{\hspace{2cm}} g}{10^{-1}g}$

USING CONVERSION FACTORS

1.11 Fill the gap in the following unit conversion:

$$20cm \times \frac{\underline{\hspace{2cm}} m}{1cm} = 0.2m$$

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

$$100\mu m \times \frac{\underline{\hspace{2cm}} m}{1\mu m} = 1 \times 10^{-4}m$$

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

$$40m \times \frac{1nm}{\underline{\hspace{2cm}}} = 4 \times 10^{-8}nm$$

1.14 Complete the following unit conversion:

$$100Gm \times \frac{\underline{\hspace{2cm}} m}{1Gm} = \underline{\hspace{2cm}} m$$

1.15 Complete the following unit conversion:

$$50km \times \frac{\underline{\hspace{2cm}} m}{1km} = \underline{\hspace{2cm}} m$$

1.16 Complete the following unit conversion:

$$2\mu m \times \frac{\underline{\hspace{2cm}} cm}{1\mu m} = \underline{\hspace{2cm}} cm$$

1.17 Complete the following unit conversion:

$$0.3\mu m \times \frac{\underline{\hspace{2cm}} mm}{1\mu m} = \underline{\hspace{2cm}} mm$$

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

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

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

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

1.20 Set up the conversion factor to convert 500cm into inches:

$$50\text{cm} \times \frac{\text{inches}}{\text{cm}} = \text{inches}$$

1.21 Set up the conversion factor to convert 400cm² into m²:

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

1.22 Compute the following power of ten calculations:

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

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

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

1.24 Fill the gap in the following conversion factors:

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

1.25 Fill the gap in the following conversion factors:

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

1.26 Complete the following unit conversion:

- | |
|---|
| (a) $0.5\mu\text{g} \times \frac{\text{g}}{\mu\text{g}} = \text{g}$ |
| (b) $125\text{L} \times \frac{\text{mL}}{\text{L}} = \text{mL}$ |

$$(c) 100\text{nm} \times \frac{\text{m}}{\text{nm}} = \text{m}$$

SIGNIFICANT FIGURES

1.27 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
- (d) The number of students in a classroom
- (e) The height of a student

1.28 Indicate the number of SFs.

- | | |
|--------------|--------------|
| (a) 0.0032 m | (d) 0.0051 m |
| (b) 5100 m | (e) 500 m |
| (c) 0.510 m | (f) 45.030 |

1.29 Which of the following numbers contains the designated CORRECT number of significant figures?

- | | |
|--------------------|--------------------|
| (a) 0.05600 (5 SF) | (d) 1.304 (2 SF) |
| (b) 0.0304 (3 SF) | |
| (c) 456 000 (3 SF) | (e) 3.12050 (4 SF) |

1.30 Carry the following calculations with the correct number of digits or significant figures:

- | | |
|----------------------|--------------------|
| (a) $0.2301 + 0.123$ | (c) $88.1 - 87.57$ |
| (b) $0.2301 - 1.12$ | (d) $24.56 + 2.4$ |

1.31 Carry the following calculations with the correct number of digits or significant figures:

- | | |
|-----------------------|------------------------|
| (a) 523×5000 | (c) 27.0×0.01 |
| (b) $5 / 0.123$ | (d) $345.13 / 100$ |

MATTER AND DENSITY

1.32 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?

- | | |
|---------------|----------------|
| (a) 10.4 g/mL | (d) 23.68 g/mL |
| (b) 6.77 g/mL | |
| (c) 1.00 g/mL | (e) 19.3 g/mL |

1.33 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)

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

1.35 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?

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

1.37 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

1.38 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?

Answers

1.1 (a) 0.33 (b) 3 (c) 0.33 (d) 1 (e) 3.5 (f) 0.5 **1.3** (a) 2 L (volume) (b) 5 cm (length) **1.5** 1×10^{-1}
1.7 1×10^{-9} **1.9** 1Tm = 10^{12} m 1dm = 10^{-1} m 1cg = 10^{-2} g 1ms = 10^{-3} s 1qt = 1mL 1L = $1dm^3$ 1lb = 454g
 $1in = 2.54cm$ **1.11** 1×10^{-2} **1.13** $1 \cdot 10^{-9}$ **1.15** $5 \cdot 10^4 m$ **1.17** $3 \cdot 10^2 mm$ **1.19** $1 \cdot 10^{-1}; 1 \cdot 10^{-2}$ **1.21** $0.04m^2$
1.23 $1cm^2 = 1 \times 10^{-4}m^2$ $1dm^3 = 1 \times 10^{-3}m^3$ $1cm^3 = 1 \times 10^{-6}m^3$ $1dm^2 = 1 \times 10^{-2}dm^2$ **1.25** $\frac{1in}{2.54cm}$
1.27 (a) The number of apples in a bag (exact) (b) The weight of an apple (measured) (c) The number of cm in a inch (exact) (d) The number of students in a classroom (exact) (e) The height of a student (measured) **1.29** 456 000 (3 SF)
1.31 (a) $523 \times 5000 = 3000000$ (b) $5/0.123 = 40$ (c) $27.0 \times 0.01 = 0.3$ (d) $345.13/100 = 3$ **1.33** balsa wood (0.16 g/mL) **1.35** 31.56mL **1.37** (a) a copper wire (Element) (b) a chocolate cookie (Homogeneous mixture) (c) a chocolate-chip cookie (Heterogeneous mixture) (d) vinegar (Homogeneous mixture) (e) ice (Compound) (f) baking soda(Compound) (g) aluminum foil(element) (h) vitamin C(compound)

PART B

2

The periodic table: atoms and Elements

MATTER is everywhere around you, from the water you drink to the air you inhale. Matter is made of elements and elements are made of atoms. Even the atoms of an elements can be different, having distinct number of protons and neutrons. This chapter covers the principles of the 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 the elements and the different types of chemical formulas.

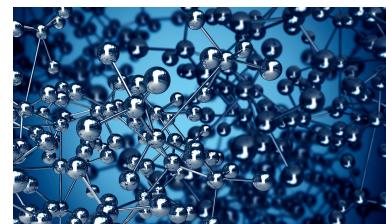
2.1 The periodic table

The periodic table 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 their name. The tabular arrangement of elements in the form of rows and columns allow 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 metals you would only find aluminium 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 exist in the element's name, the second letter should be lowercase. For example, the chemical symbol for aluminum is Al with capital A and lowercase l. The periodic table in next page contains the symbols of all elements.

Periods and groups The periodic table 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). The groups numbers can be found written with roman numbers and a letters (A or B) or with a more modern group numbering of 1-18 going across the periodic table. For example, the group 2 (Mg-Ra) can also be called IIA, and the group 13 (B-Ti) is also known as IIIA.



185

GOALS

- 1 Navigate the periodic table
- 2 Calculate the number of electrons, protons and neutrons in an atom
- 3 Calculate average atomic masses
- 4 Calculate simple molecular weights
- 5 Calculate molecular formulas from empirical formulas

190

195

 **Discussion:** Why having a periodic table? What is the basic information all periodic tables provide? Do you know any other periodic table design?

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205

210

215

 Nothing exists except atoms and empty space; everything else is opinion.

Democritus



Properties in the periodic table The physical and chemical properties of some elements of the table 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.

The periodic table displays the following information for each element:

- Atomic Number (Z):** The element's position in the table.
- Symbol:** The standard one- or two-letter symbol for the element.
- Name:** The full name of the element.
- Mass:** The atomic mass of the element.
- Category:** A color-coded classification based on element type:
 - Alkali Metal:** Group 1 (Li, Na, K, Rb, Cs, Fr)
 - Alkaline Earth Metal:** Group 2 (Be, Mg, Ca, Sr, Ba, Ra)
 - Transition metals:** Groups 3-12 (Sc-Tm, Hf-Lu, Ac-Lr)
 - Metalloid:** Groups 13-15 (B, Si, Ge, As, Sb, Te, Po, At)
 - Chalcogen:** Groups 16-17 (O, S, Se, Te, Po)
 - Halogen:** Groups 17-18 (F, Cl, Br, I, At)
 - Noble Gas:** Group 18 (He, Ne, Ar, Kr, Xe, Rn, Uuo)
 - Lanthanide/Actinide:** Lanthanides (Ce-Lu) and Actinides (Ac-Lr)

Figure 2.1 The periodic table of the elements

Metals, Nonmetals, and Metalloids Overall, the elements of the periodic table 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 the nonmetals. For example, they are better conductors of heat and electricity than the nonmetals, but not as good conductors as the metals. Metalloids are semiconductors because they can act as both conductors and insulators under certain conditions. An example of metalloids is Silicon (Si) that should not be confused from silicone, a chemical employed in prosthetics.

Classification of elements in terms of groups Some of the groups in the periodic table 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 the group 2A (2) elements: beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba), and radium (Ra). Transition metals are the elements from group 3 to 12 and they are located in the middle of the table. Chalcogens are the group 6A (16) elements: oxygen (O), sulfur (S), selenium (Se), tellurium (Te), and polonium (Po).

Halogens are the group 7A (17) elements: fluorine (F), chlorine (Cl), bromine (Br), iodine (I), and astatine (At). Halogens are very reactive elements. Finally, noble gases are the 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 meet a royal? 250

How to classify Hydrogen At first sight, hydrogen (H) may seem to be put in the wrong spot at the periodic table. 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 a nonmetal. 255

Sample Problem 13

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

SOLUTION

(a) The chemical symbol of Au is Gold. The chemical symbol of Iron is Fe and the chemical symbol of Iodine is I. (b) 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. (c) 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. (d) Ba (Barium) is a metal. N (Nitrogen) is a nonmetal. Si (Silicon) is a metalloid.

❖ STUDY CHECK

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

Answer: (a) Nickel; (b) Chlorine: G 17 (VIIA) P3; (c) Neon Noble gas ; (d) Tungsten metal.

2.2 The atom

260

Atoms are the smallest piece of an element that retains its 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 elements are not equal.

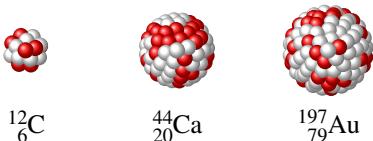
Atomic Structure Atoms contain three atomic particles: the proton, neutron, and electron. Protons have positive charge (+), whereas electrons carry negative charge (−). Neutrons on the other hand are neutral, and they have no electrical charge. Protons and neutrons are located in the core of the atom, which is called the nucleus, and account for the mass of the atom. 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 265 270

area next to the nucleus. When an atom is neutral it has no charge and the number of electrons and protons are the same. Some atoms have positive charge, resulting of removing electrons, and we call these cations. Others—called anions—can have negative charge as a result of accepting a negatively charged electron.

²⁷⁵ *Atomic and mass number* Elements are made of atoms, and each atom of an element is characterized by a atomic number (Z) and a mass number (A). The atomic number (Z) of an element indicates the number of electrons of an atom. This number can be easily located in the periodic table. The mass number (A) of an element indicates the combined number of protons and neutrons. Mass numbers are nowhere located ²⁸⁰ in the periodic table as different atoms of the same element can have different mass numbers. Both A and Z for an atom X are indicated in the following form called isotope notation:



²⁸⁵ As an example, the notation ${}^{24}_{12} \text{Mg}$ means that the atomic number of Mg is $Z=12$ and the mass number is $A=24$. Remember that the atomic number can be found in the periodic table whereas the mass number A is not on the table. By means of 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 ²⁹⁰ 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.



Sample Problem 14

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) ${}^{36}_{16} \text{S}$

Answer: (a) 16p, 16e and 16n; (b) 16p, 16e and 18n; (c) 16p, 16e and 20n.

²⁹⁵ *Isotopes* All atoms of the same element are not the same. Some are heavier than others. Isotopes are atoms of the same element with different numbers of neutrons and therefore with different mass number 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. Each of the isotopes has a specific abundance, as some isotopes are more abundant than others. For example, the abundance of ${}^{24}_{12} \text{Mg}$ is

79%, and the abundance of ^{25}Mg and ^{26}Mg is 10% and 11%, respectively. This means, 300
 ^{24}Mg is more abundant than for example ^{26}Mg .

Average atomic mass The average atomic mass represents the mass of the atoms of an element and results from all existing isotopes taking into account their abundance. The units of atomic mass are called *amu*, which stands for atomic mass units. This value can be simply found at any periodic table. Using the periodic table provided in this manual Figure??, you can find the atomic mass of each element on top of the symbol at the right side. For example, the atomic mass of oxygen (O) is 15.999 amu and the atomic mass of nitrogen (N) is 14.007 amu. As atoms are made of numerous isotopes—this means different atoms of the same element but with different number of neutrons and hence different weight—the atomic mass found in the periodic table is an average that result from including the mass of the different isotopes and their abundance. That is you need to do an average of the mass of each isotope using values of abundance. In another words: the *average atomic mass* of an element—herein called simply atomic mass—, expressed in *amu* (atomic mass units), is the weighted average of the masses of the individual isotopes of the element. For an element with n isotopes with different masses (A_1, A_2, \dots, A_n) and different fractional abundances for each isotope (f_1, f_2, \dots, f_n), the atomic mass is given by 305

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

Also, note that when adding the fractional abundances of all isotopes, one should obtain a value of one: 310

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

Sample Problem 15

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? 315

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:

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

❖ 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 copper's atomic weight is 6.94 amu.

Answer: 7.59% and 92.41%. 320

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%
	^{18}O	0.205%		^{41}K	6.7302%

2.3 An introduction to molecules

The periodic table 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 form the molecule taking into account the number of atoms of each element present in the molecule.

Units of molecular weight The units of molecular weight are the same as the units of atomic weight: amu, atomic mass units.

Sample Problem 16

Calculate: (a) The atomic weight of O; (b) the molecular mass of molecular oxygen, O_2

SOLUTION

- (a) According to the periodic table the atomic weight (AW) of O is 15.999 amu.
- (b) The molar mass of O_2 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

Answer: 18 and 17 amu.

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 by means of the mass % composition. The mass % of an element in a compound is the mass of the element with respect to 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:

345

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

Similarly, the mass % of C would be:

350

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

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 17

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 %_C 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.

Answer: 20%_C, 26.7%_O, 46.7%_N, 6.6%_H.

2.4 Empirical and molecular formula of a chemical

There are two different types of formulas: molecular formulas and empirical formulas. Empirical formula (EFs) are simplified formulas resulting from an experiment, whereas molecular formulas (MFs) are exact formulas of molecules. For example: the molecular

355

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 actually come from experiments, and from experiments one normally can only obtain ratios of atomic composition.

Sample Problem 18

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 $\text{C}_6\text{H}_{18}\text{O}_3$.

Answer: P_2O_5 , NO_2 and $\text{C}_2\text{H}_6\text{O}$.

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 a integer number such as 1, 2, 3...

370

375

Understanding the formula above is simple. On one hand, the MW of a molecular formula H_2O_2 that 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 in order 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 molecular formula in mind. Let us work on an example:

Sample Problem 19

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

SOLUTION

Given the empirical formula of dichloromethane 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 weigh of the chemical is 92 amu. Calculate the molecular formula of dinitrogen tetroxide.

Answer: N_2O_4 .

2.5 Determining empirical formulas

380

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 is 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 in order to learn the procedure of obtaining molecular formulas.

385

Calculating molecular formulas By means of a experiment, 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. In order to calculate the EF we will set up a table like the one presented below.

390

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

395

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 20

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?

Answer: CH_2O .

CHAPTER 2

2.1 Select from below the atomic symbol for the element Gold is:

- | | | |
|--------|--------|--------|
| (a) Go | (c) G | (e) Ol |
| (b) Au | (d) Ca | |

2.2 The atomic symbol for aluminum is:

- | | | |
|--------|--------|--------|
| (a) Al | (c) A | (e) Ag |
| (b) Am | (d) Sn | |

2.3 The atomic symbol for iron is:

- | | | |
|--------|--------|--------|
| (a) Ir | (c) Fe | (e) Ir |
| (b) Fs | (d) In | |

2.4 Ca is the symbol for:

- | | |
|-------------|-------------|
| (a) Carbon | (d) Copper |
| (b) Calcium | |
| (c) Cobalt | (e) Cadmium |

2.5 Which of the following elements is a metal?

- | | |
|--------------|------------|
| (a) Nitrogen | (d) Iron |
| (b) Lithium | |
| (c) Calcium | (e) Iodine |

2.6 Which of the following elements is a alkaline metal?

- | | |
|--------------|---------------|
| (a) Nitrogen | (d) Iron |
| (b) Lithium | |
| (c) Calcium | (e) Ruthenium |

2.7 Which of the following elements is a nonmetal?

- | | |
|--------------|------------|
| (a) Nitrogen | (d) Iron |
| (b) Lithium | |
| (c) Calcium | (e) Iodine |

2.8 Which of the following elements is a halogen?

- | | |
|--------------|------------|
| (a) Nitrogen | (d) Iron |
| (b) Lithium | |
| (c) Calcium | (e) Iodine |

2.9 What is the symbol of the element in Period 4 and Group 2?

- | | |
|--------|--------|
| (a) Be | (d) C |
| (b) Mg | |
| (c) Ca | (e) Si |

THE ATOM

2.10 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.

2.11 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

2.12 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

2.13 The mass number of an atom is equal to the number of

- (a) electrons
- (b) neutrons
- (c) neutrons plus protons.
- (d) protons

2.14 Consider a neutral atom with 30 protons and 34 neutrons. The atomic number of the element is

- | | |
|--------|--------|
| (a) 30 | (d) 64 |
| (b) 32 | |
| (c) 34 | (e) 94 |

2.15 Consider a neutral atom with 30 protons and 34 neutrons. The mass number of the element is

- | | |
|--------|--------|
| (a) 30 | (d) 64 |
| (b) 32 | |
| (c) 34 | (e) 94 |

2.16 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.

AN INTRODUCTION TO MOLECULES

2.17 Calculate the molecular mass of the following molecule: CCl_2F_2

2.18 Calculate the molecular mass of the following molecule: C_4H_{10}

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

EMPIRICAL AND MOLECULAR FORMULAS

2.20 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?

2.21 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=60amu

2.22 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.

2.23 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.

Answers **2.1** (b) **2.3** (c) **2.5** (d) **2.7** (a) **2.9** (c) **2.11** (e) **2.13** (c) **2.15** (d) **2.17** 121 amu **2.19** 210 amu
2.21 CH_2O **2.23** NO_2

3

Chemical naming

ALL elements in the periodic table with the exception of the noble gases—He, Ne, Ar, Kr, Xe and Rn—combine to produce chemical compounds. Most of these chemicals are useful in your every day 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 to 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 loose 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 the ionic charges.

Cations Atoms that loose electrons become positively charged. These ions are called cations. Example of cations are Li^+ or Mg^{2+} called lithium cation and magnesium cation, respectively.

Anions Atoms that gain electrons become negatively charged, as electrons have negative charge. These ions are called anions. Example 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.

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 ionic charges, and the numbers are coming from the periodic table. H, Na or K are in the group IA (left of the table) and hence the ionic charge will be $1+$. Similarly, Mg or Ca are in the group IIA (left of the table) and hence the ionic charge will be $2+$. Differently, F, Cl or Br are in the group 7A (right of the table) and its charge will be $1-$. Oxygen is in group 6A (right of the table) and the ionic charge will be $2-$. Figure 3.1 contains all ionic charges. What if the element is not in this list such as the case of Iron (Fe)? In that case,



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GOALS

- 1 Name and formulate ionic compounds
- 2 Name and formulate covalent compounds
- 3 Name and formulate acids and bases
- 4 Name and formulate oxosalts
- 5 Name and formulate common chemicals

415

Discussion: think about your household and the chemicals you use at home. List three chemicals you found around you, with its correct chemical name

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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 3.1 as iron can have several ionic charges.

440

Sample Problem 21

Identify the correct ionic state of: Cl, K, O and 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⁺, O²⁻ and C⁴⁻.

◆ STUDY CHECK

Identify the correct ionic state of: N and Br.

Answer: N³⁻ and Br⁻.

Figure 3.1: Ionic charges (valences) for different elements

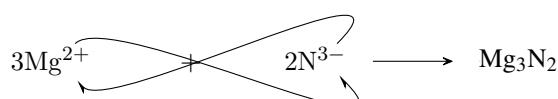
		18 VIIA																									
		1 IA		2 IIA																							
		Li ⁺		Be ²⁺																							
		Na ⁺		Mg ²⁺																							
		K ⁺		Ca ²⁺		3 IIIB		4 IVB		5 VB		6 VIB		7 VIIB		8 VIIIIB		9 VIIIB		10 VIIIIB		11 IB		12 IIB			
		Rb ⁺		Sr ²⁺								Cr ²⁺ Cr ³⁺		Mn ²⁺ Mn ³⁺		Fe ²⁺ Fe ³⁺		Co ²⁺ Co ³⁺				Cu ⁺ Cu ²⁺		Zn ²⁺		Ga ³⁺	
		Cs ⁺		Ba ²⁺																		Sn ²⁺ Sn ⁴⁺					
																						Pb ²⁺ Pb ⁴⁺					

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 of combining sodium (a metal) with chloride (a non metal).

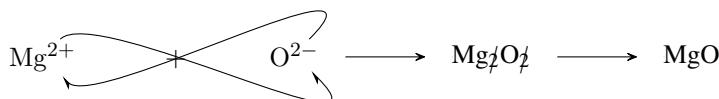
Combining ions Ionic compounds are the result of combining two ions: a positive (cation) and a negative (anion) ions. Each ion has a charge, depending on its location on the table. When combining two atoms you first need to arrange the ions starting from positive and followed by negative. The charges of an ion would become the coefficient of the other ion. For example Mg²⁺ and N³⁻ are combined as Mg₃N₂:

445



Another example would be the combination of Na⁺ and O²⁻ that would be Na₂O. You need to simplify the indexes of the formula by diving by the smallest one, always using integer values. For example, Mg²⁺ and O²⁻ give Mg₂O₂ that should be written as MgO

455



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

Sample Problem 22

Combine the following ions or give the ions given the final compound:

Ions	Combination
Li^+ and O^{2-}	Li_3N
Ca^{2+} and O^{2-}	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: Na^+ and F^- and Na_3N .

Answer: NaF ; Na^+ and N^{3-} .

460

Simple ionic naming (type I ionic) Type I ionic compounds result from the combination of a metal with given valence (Li, Ca, Mg, etc.) and a non metal. In order 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 as sodium chloride and MgCl_2 is named magnesium chloride. Another example would be:

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CaCl₂ calcium chlorideLiO₂

lithium oxide

465

In order 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 of 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:

470



The sign of the charges only indicate which element goes first in the formula: the positive element (cation) first following by the negative element (anion). For example

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the result of combining Na^+ and Cl^- is NaCl and not ClNa as Na has positive ionic charge and has to appear first in the formula.

Sample Problem 23

Name or give the formula for the following ionic compounds:

Formula	Name
MgO	
Mg_3N_2	Lithium nitride 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: Sodium fluoride and Na_3N .

Answer: NaF ; Sodium nitride.

Complex ionic naming The ionic chemical NaCl results from the combination of Na^+ and Cl^- . The ionic charges of Na and Cl are given in Figure 3.1 according to the group. If the ionic chemical contains a transition metal with variable ionic charge, that is, which is not in Figure 3.1 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.

Formulate complex ionic chemicals In this section we will learn how to name ionic chemicals containing a metal with several possible charges, that is a metal which is not included in Figure 3.1. The charge of the metal has to be given in the name. As an example, the formula for Nickel(III) oxide is Ni_2O_3 . The reason for the formula is the combination of Nickel(III) Ni^{3+} and oxygen O^{2-} , that gives Ni_2O_3 , after crossing the charges from top to bottom. Another example is Nickel(II) oxide formulated as NiO . This results from combining Nickel(II) Ni^{2+} and oxygen O^{2-} that gives Ni_2O_2 . After simplifying one obtains NiO .

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. In order 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 3.1, lets 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 at normal conditions. A typical ionic compound would be NaCl , cooking salt.

The ionic bond Atoms of an ionic compound are connected by means of 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.

510

Sample Problem 24

Name or give the formula for the following ionic compounds:

Formula	Name
MnO	
Fe_3N_2	
Cobalt(II) carbide	
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: Manganese(IV) oxide and AuCl.

Answer: MnO_2 ; Gold(I) chloride.

3.3 Covalent compounds

Covalent compounds are chemicals resulting from the combination of nonmetallic elements. An example is CO_2 , which results of combining carbon (a non metal) with oxygen (a non metal).

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Covalent naming In order 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 that indicate the number of atoms in the molecule. See Table 3 for a list of the different equivalencies between prefixes and number. As an example, the formula CH_4 is named as 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

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525

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:

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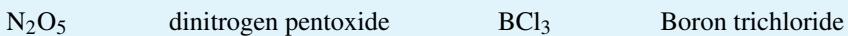


Table 3.1 Prefixes used to name covalent compounds

Prefix	number	Prefix	number
Mono	1	Hexa	6
Di	2	Hepta	7
Tri	3	Octa	8
Tetra	4	Nona	9
Penta	5	Deca	10

Sample Problem 25

Name of give the name of the following covalent chemicals:

Formula	Name
NO	
CS_2	Sulfur Dioxide
	Nitrogen Trichloride

CS_2	Sulfur Dioxide
	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 oxide. CS_2 is called carbon disulfide. The formula for sulfur dioxide and nitrogen trichloride are respectively SO_2 and NCI_3 .

❖ STUDY CHECK

Name of give the name of the following covalent chemicals: SCl_2 and diboron thrioxide.

Answer: sulfur dichloride and B_2O_3 .

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Properties of covalent compounds 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.

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The covalent bond 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.

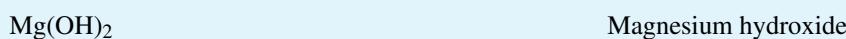
3.4 Naming acids & bases

In this section we will learn how to name acids and bases. Acids normally have common names (e.g. sulfuric acid) and its 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.

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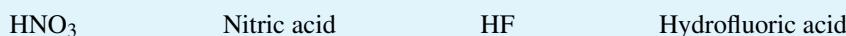
Bases or hydroxides Bases (hydroxides) result from the combination of a metal and the hydroxide anion (OH^-). Examples are NaOH or $\text{Ca}(\text{OH})_2$. The name of a base starts by the name of the cation finishing by the word *hydroxide*. An example is NaOH named as *sodium hydroxide*, or $\text{Ca}(\text{OH})_2$, 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:

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Acids Acids—in particular inorganic acids—are chemicals that normally contain hydrogen at the beginning of its formula. For example, HCl or H_2SO_4 . HCl is an 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 3.2 contains a list of the most important oxoacids and hydracids. More examples of acids:

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Sample Problem 26

Name or give the formula for the following acids and bases. Indicate whether the compound is an acid or a base.

Formula	Acid/Base	Name
HCN		
KOH		
	Carbonic acid	
	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: phosphoric acid and $\text{Mg}(\text{OH})_2$.

Answer: H_3PO_4 ; magnesium hydroxide.

Oxidation states of oxoacids Consider the following set of acids: HClO, HClO₂, HClO₃ and HClO₄. We say Cl in these acids have different oxidation state or different oxidation number. 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 underline element, Cl. In order to do this we will follow a set of simple rules. First, we will use the valences as the oxidation number of the elements to the right and to 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 a equation so that the sum of all oxidation numbers equals to 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 an oxoacid results from the fact that acids with high or low oxidation states, tends to be very reactive, being sometimes capable of completely dissolving metals. We call these oxidizing (or reducing) acids. For example, HNO₃ and H₂SO₄ and 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 acid sor agents. Let us compare two oxoacids in order 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 27

Calculate the redox number of S in the following acids and indicate the more oxidizing acid: H₂S₂O₆ named dithionic acid and H₂SO₄ named sulfuric acid.

SOLUTION

We will set up the redox formula for the first acid (H₂S₂O₆), 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 H₂S₂O₃ is +5. For the second acid (H₂SO₄):

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

Solving for x:

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

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: H_2MnO_4 and $\text{H}_2\text{Cr}_2\text{O}_7$.

Answer: +6.

595

Table 3.2 Names of oxoacids and oxosalts (top table) and hyracids (bottom table). Yellow rows need to be remembered.

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
	$\text{H}_2\text{S}_2\text{O}_2$	Thiosulfurous Acid	$\text{S}_2\text{O}_2^{-2}$	Thiosulfite
	$\text{H}_2\text{S}_2\text{O}_3$	Thiosulfuric Acid	$\text{S}_2\text{O}_3^{-2}$	Thiosulfate
	$\text{H}_2\text{S}_2\text{O}_7$	Disulfuric acid	$\text{S}_2\text{O}_7^{-2}$	Disulfate
Chlorine	$\text{H}_2\text{S}_2\text{O}_8$	Peroxodisulfuric acid	$\text{S}_2\text{O}_8^{-2}$	Peroxodisulfate
	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
	$\text{H}_2\text{Cr}_2\text{O}_7$	Dichromic acid	$\text{Cr}_2\text{O}_7^{2-}$	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	

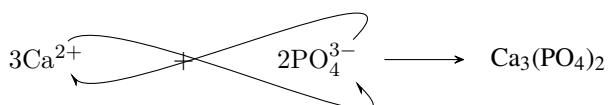
3.5 Naming complex salts & common chemicals

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

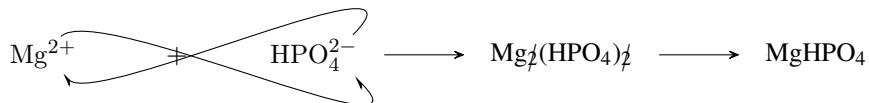
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they have at least three different elements. An example of oxosalt would be CaSO_4 called calcium carbonate. An example of hydrosalt would be NaHSO_4 which is called sodium monohydrosulfate. This section will also cover the naming of hydrates (e.g. $\text{CaSO}_4 \cdot \text{H}_2\text{O}$),
605 that are compounds containing water molecules inside its structure. Before being able to name these complex chemicals it is convenient to practice combining ions, without paying attention to the naming.

Combining ions In order to combine two ions, you first arrange the positive ion in
610 the left followed by the negative ion in 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 $\text{Ca}_3(\text{PO}_4)_2$:



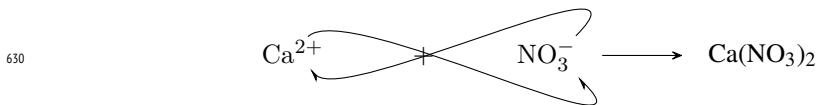
We would simplify in case the charges compensate with each other. An example would
615 be combining Mg^{2+} and HPO_4^{2-} leading to MgHPO_4



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
620 3.2. For example, the name of MgSO_4 is magnesium sulfate, as Mg^{2+} is magnesium and SO_4^{2-} is sulfate. Another example is $\text{Fe}_2(\text{CO}_3)_3$ called Iron(III) carbonate. A final example:

NO_3^-	Nitrate	LiNO_3	Lithium nitrate (oxosalt)
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Formulating Oxosalts In the case that you know the name of an oxosalt and you
625 want to obtain its formula, you first need to arrange the positive ion in the left followed by the negative ion in 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 28

Name of give the name of the following oxosalts:

Formula	Name
K ₂ SO ₄	
Na ₂ CO ₃	
	Nickel(II) carbonate
	Sodium phosphate

SOLUTION

K₂SO₄ is named potassium sulfate, as K⁺ is potassium and SO₄²⁻ stands for sulfate. Na₂CO₃ is sodium carbonate. Nickel(II) carbonate is NiCO₃ and sodium phosphate is Na₃PO₄.

◆ STUDY CHECK

Name of give the name of the following oxosalts: FeSO₄ and Iron(III) sulfate.

Answer: Iron(II) sulfate and Fe₂(SO₄)₃.

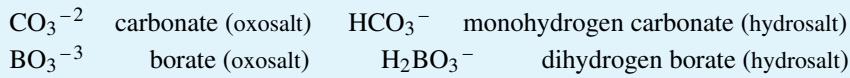
Naming Hydrosalts Hydrosalts are related to oxosalts (e.g. Na₂SO₄) and they resemble these chemicals while having hydrogen atoms in their chemical formula, in between the oxosalt cation and anion (e.g. NaHSO₄). That is the reason they are called hydrosalts as they are oxosalts with hydrogen. For example, NaHSO₄ is named sodium monohydrogensulfate. In order to understand this name, we will first focus on the second part on the name, monohydrogensulfate that represents the hydrosalt anion.

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The name monohydrogensulfate (HSO₄⁻) comes from adding a proton (H⁺) to a sulfate cation (SO₄²⁻). Mind that protons (H⁺) are positively charged and therefore if we add a single H⁺ to a sulfate cation (SO₄²⁻) the charge will have to decrease a single unit, giving us HSO₄⁻. As we can see, the name of hydrosalt anions are directly related to the oxosalt anion and the number of hydrogens in the hydrosalt name. For example, phosphate (PO₄³⁻) is an oxosalt anion whereas hydrogenphosphate (HPO₄²⁻) and dihydrogenphosphate (H₂PO₄⁻) 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 hast to have two less negative charges (that is -1). Some final hydrosalt anions examples:

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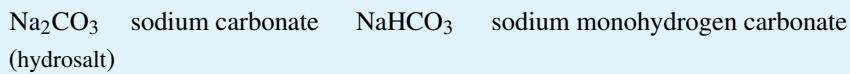
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Above we saw how to name just the ending of the hydrosalt. Now we can move forward to the naming of hydrosalts. We just need to add the name of the element in the first place, and for example NaH₂BO₃ would be named sodium dihydrogenborate. If the first 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, Fe(H₂BO₃)₂ would be named iron(II) dihydrogenborate. More examples:

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Sample Problem 29

Name or formulate the following hydrosalts:

Formula	Name
	Magnesium hydrogensulfate
	Sodium hydrogen carbonate
LiHCO_3	
MgH_2PO_4	

SOLUTION

The formula of Magnesium hydrogensulfate is $\text{Mg}(\text{HSO}_4)_2$ as the formula for monohydrogen sulfate is HSO_4^- and the valence of magnesium is Mg^{2+} . The formula for Sodium monohydrogen carbonate is NaHCO_3 as it results from combining Na^+ and HCO_3^- . Mind monohydrogen carbonate results from adding a hydrogen ion H^+ to a carbonate CO_3^{2-} ion. The name for LiHCO_3 is lithium monohydrogen carbonate, whereas the name for MgH_2PO_4 is magnesium dihydrogenphosphate.

◆ STUDY CHECK

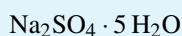
Name or formulate the following hydrosalts: LiHS_2O_3 , LiH_2PO_4 and sodium hydrogenphosphate.

Answer: lithium monohydrogenthosulfate; Lithium dihydrogenphosphate and Na_2HPO_3 .

660

665

Hydrates Some chemicals contain water molecules trapped in its structure and therefore water molecules (H_2O) are often indicated in chemical formulas. These types of chemicals containing water are called *hydrates*, precisely because hydrate means water. Examples of hydrates are: $\text{BeSO}_4 \cdot 4 \text{H}_2\text{O}$ or $\text{CuSO}_4 \cdot 5 \text{H}_2\text{O}$ called respectively beryllium sulfate tetrahydrate and copper(II) sulfate pentahydrate. In order to formulate hydrates you just need to use prefixes such as mono, di, tria—the same ones we use to name covalent chemicals—to indicate the number of water molecules in the chemical and end the name with *hydrate*. As a note, warming up hydrates (e.g. $\text{BeSO}_4 \cdot 4 \text{H}_2\text{O}$) results on the release of water producing a dehydrated or *anhydrous* compound (e.g. BeSO_4). A final example of hydrate naming:



(a hydrate)

Sodium sulfate pentahydrate

Sample Problem 30

Name or formulate the following hydrates:

Formula	Name
	Nickel(II) permanganate dihydrate
	Sodium nitrate monohydrate
$\text{Na}_2\text{CO}_3 \cdot 10 \text{H}_2\text{O}$	
$\text{MgSO}_4 \cdot 7 \text{H}_2\text{O}$	

SOLUTION

The formula for Nickel(II) permanganate is $\text{Ni}(\text{MnO}_4)_2$, therefore the formula for Nickel(II) permanganate dihydrate is $\text{Ni}(\text{MnO}_4)_2 \cdot 2 \text{H}_2\text{O}$. The formula for Sodium nitrate is NaNO_3 , therefore $\text{NaNO}_3 \cdot \text{H}_2\text{O}$ is Sodium nitrate monohydrate. The name for $\text{Na}_2\text{CO}_3 \cdot 10 \text{H}_2\text{O}$ is sodium carbonate decahydrate and $\text{MgSO}_4 \cdot 7 \text{H}_2\text{O}$ is magnesium sulfate heptahydrate.

❖ STUDY CHECK

Name or formulate the following hydrates: $\text{LiNO}_3 \cdot \text{H}_2\text{O}$, $\text{Na}_3\text{PO}_4 \cdot 3 \text{H}_2\text{O}$ and sodium sulfate tetrahydrate.

Answer: lithium nitrate monohydrate; sodium phosphate trihydrate and $\text{Na}_2\text{SO}_4 \cdot 4 \text{H}_2\text{O}$.

670

Common naming Some of the chemicals are normally referred by a common name that does not involve the use of any chemical naming rules. An example would be H_2O normally referred as water instead of its standard name that is dihydrogen oxide. You can find more names in Table 3.3. Another example:

675

NaCl	Sodium chloride (standard name)	Table salt (common name)
------	---------------------------------	--------------------------

Table 3.3 List of common chemicals

Chemical	Name	Chemical	Name
H_2O	Water	$\text{Mg}(\text{OH})_2$	Milk of magnesia
NH_3	Ammonia	N_2O	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	$\text{MgSO}_4 \cdot 7 \text{H}_2\text{O}$	Epsom Salt

Sample Problem 31

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

SOLUTION

The formula for milk of magnesia is $\text{Mg}(\text{OH})_2$ (magnesium hydroxide), whereas dry ice is the common name for CO_2 , carbon dioxide.

❖ STUDY CHECK

Name or formulate the following common chemicals: ammonia and methane.

Answer: NH_3 (nitrogen trihydride) and CH_4 (carbon tetrahydride).

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 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

COVALENT COMPOUNDS

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

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

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

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

IONIC COMPOUNDS

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

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

3.9 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

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

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

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

ACIDS AND HYDROXIDES

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

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

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

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

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

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

3.19 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

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

3.21 Identify the most oxidated acid:

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

3.22 Identify the most reduced acid:

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

3.23 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 OXOSALTS

3.24 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

3.25 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

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

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

HYDROSALTS, HYDRATES & COMMON CHEMICALS

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

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

3.30 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 (c) $\text{KMnO}_4 \cdot 4\text{H}_2\text{O}$ (d) Lithium sulfate tetrahydrate

3.31 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

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

GENERAL PROBLEMS

3.33 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

3.34 Name the following compounds:

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

3.35 Combine the following ions:

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

3.36 Memorize the following oxoacids:

- | |
|---|
| (a) H_2SO_4 Sulfuric acid |
| (b) H_2CO_3 Carbonic acid |
| (c) HMnO_4 Permanganic acid |
| (d) HNO_3 Nitric acid |
| (e) H_3PO_4 Carbonic acid |
| (f) $\text{H}_2\text{Cr}_2\text{O}_7$ Dicromic acid |

3.37 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 |

3.38 Formulate the following compounds:

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

3.39 Name the following compounds:

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

3.40 Combine the following polyatomic ions:

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

3.41 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

3.42 Combine the following ions:

- | | |
|---------------------------------------|---------------------------------------|
| (a) $\text{Cs}^+ + \text{Ni}^-$ | (d) $\text{Li}^+ + \text{Cu}^-$ |
| (b) $\text{Sr}^{2+} + \text{Mn}^{2-}$ | |
| (c) $\text{Be}^{2+} + \text{Co}^{4-}$ | (e) $\text{Mg}^{2+} + \text{Cr}^{-6}$ |

3.43 Formulate the following compounds:

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

3.44 Name the following compounds:

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

3.45 Name the following compounds:

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

3.46 Name or formulate the following oxoanions:

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

3.47 Combine the following ions:

- | | |
|--------------------------------------|--|
| (a) $\text{Na}^+ + \text{PO}_4^{3-}$ | (d) $\text{Ca}^{2+} + \text{CO}_3^{2-}$ |
| (b) $\text{Li}^+ + \text{MnO}_4^-$ | (e) $\text{Cs}^+ + \text{Cr}_2\text{O}_7^{2-}$ |
| (c) $\text{Mg}^{2+} + \text{NO}_3^-$ | (f) $\text{K}^+ + \text{BO}_3^{3-}$ |

3.48 Name or formulate the following compounds:

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

3.49 Name or formulate the following compounds:

- | | |
|----------------------------------|-------------------------------|
| (a) MnSO_4 | (d) $\text{V}(\text{NO}_2)_2$ |
| (b) CuNO_3 | |
| (c) $\text{Cr}_2(\text{CO}_3)_3$ | (e) FeSO_3 |

3.50 Name or formulate the following pairs or ions:

- | | |
|--|--|
| (a) carbonate and mono-hydrogencarbonate | (d) phosphate and dihydrogenphosphate |
| (b) sulfate and monohydrogensulfate | (e) phosphate and mono-hydrogenphosphate |
| (c) cromate and monohydrogenchromate | (f) borate and dihydrogenphosborate |

Answers

3.1 (a) Fe^{2+} (cation) (b) Cl^- (anion) (c) Ag (atom)

3.3 (a) NO (nitrogen monoxide) (b) Dichlorine monofluoride (Cl_2F) (c) NO_2 (nitrogen dioxide)

3.5 (a) SO_3 (sulfur trioxide) (b) Disulfur dichloride (S_2Cl_2) (c) SO_2 (sulfur dioxide) (d) Disulfur tetrachloride (S_2Cl_4)

3.7 (a) Magnesium iodide (MgI_2) (b) Ca_3P_2 (Calcium phosphide) (c) Lithium nitride (Li_3N) (d) MgF (Magnesium fluoride)

3.9 (a) Fe_3P_2 (Iron(II) phosphide) (b) Copper(II) iodide (CuI_2) (c) Fe_3N_2 (Iron(II) nitride) (d) Iron(II) sulfide (FeS)

3.11 (a) FeI_2 (Iron(II) iodide) (b) Lead(IV) sulfide (PbS_2) (c) FeBr_2 (Iron(II) bromide)

3.13 (a) HCl (hydrochloric acid) (b) Hydrofluoric Acid (HF) (c) Mg(OH)_2 (magnesium hydroxide)

3.15 (a) KOH (base) (b) LiOH (base) (c) CH_3OH (acid, organic)

3.17 (a) HF (hydracid) (b) H_2SO_3 (oxacid) (c) H_2S (hydracid)

3.19 (a) H_2CrO_4 redox=6 (b) $\text{H}_2\text{Cr}_2\text{O}_7$ redox=6 (c) HMnO_4 redox=7

3.21 (a) $\text{H}_3\text{As}^{\text{V}}\text{O}_4$ (b) $\text{H}_4\text{Xe}^{\text{VIII}}\text{O}_6$

3.23 (a) $\text{H}_2\text{S}_2^{\text{V}}\text{O}_6$ (b) $\text{H}_2\text{Se}^{\text{IV}}\text{O}_3$

3.25 (a) Lithium sulfate (Li_2SO_4) (b) Na_2CrO_4 (sodium dichromate) (c) Lithium sulfite (Li_2SO_3) (d) $\text{Cs}_2\text{Cr}_2\text{O}_7$ (caesium dichromate) (e) Calcium sulfate (CaSO_4)

3.27 (a) cobalt(III) carbonate ($\text{Co}_2(\text{CO}_3)_2$) (b) $\text{Fe}(\text{ClO}_4)_3$ (iron(III) perchlorate) (c) zinc(II) carbonate (ZnCO_3)

3.29 (a) Sodium dihydrogenphosphate (NaH_2PO_4) (b) LiH_2PO_4 (lithium dihydrogenphosphate) (c) Silver monohydrogenphosphate (Ag_2HPO_4)

3.31 (a) MgSO_4 (magnesium phosphate) (b) $\text{Ni}(\text{SO}_4)_3$ (nickel(III) sulfate) (c) Cobalt(II) nitrate ($\text{Co}(\text{NO}_3)_2$) (d) Cobalt(II) sulfate dihydrate ($\text{CoSO}_4 \cdot 2\text{H}_2\text{O}$) (e) KHCO_3 (potassium monohydrogencarbonate)

PART C

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

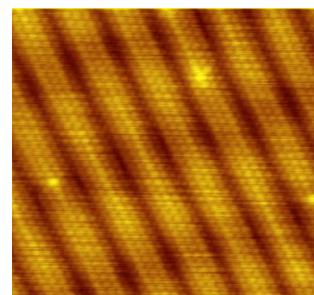
Some of the terms you use in your everyday life actually refer to a number. For example, you buy a pair of socks—two socks—or you buy a dozen of eggs from the grocery store—twelve eggs—and sometimes you buy a case of beers—24 cans. In a chemistry laboratory we normally do not weight small numbers of 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, in reference to 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 the 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 mole is mol, and for example we will say seven mol of H₂O.

From moles to atoms 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 follow 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:

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



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GOALS

- 1 Transform grams into moles and moles into molecules
- 2 Balance chemical reactions
- 3 Carry stoichiometric calculations
- 4 Identify the limiting reagent
- 5 Calculate the % yield

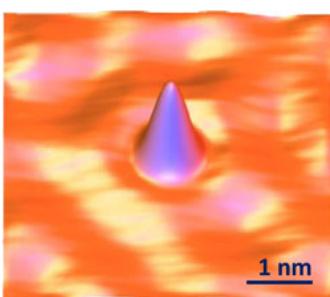
695

Discussion: What weights more one kilo of Sulfur or one kilo of Gold? Now, what weights more, one mol of Sulfur or one mole of Gold

700

705

▼Molecules are counted by the mole



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▼Eggs are bought by the dozen



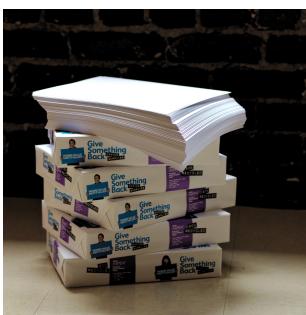
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▼Socks are bought as pairs



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▼A ream of paper contains 500 sheets



© wikipedia

▼A six-pack contains 6 beers



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▼A gross is a dozen of dozens



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Figure 4.1: Collections of items and their name

For example: how many molecules are there in 3 mol of H_2O ? In order to calculate the number of molecules of H_2O in 3 moles of H_2O , (moles → molecules) you need to set up a conversion factor, starting by the give information (3 moles) and using the mol-to-molecule conversion factor with mol on the bottom:

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

In 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 molecule in the bottom. For example 3×10^{20} H_2O molecules equals to 4.98×10^{-4} moles of H_2O as

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

From molecules to atoms Molecules are made of atoms, and for example the CO_2 molecule contains an atom of C and two atoms of O. In order to convert from molecules to atoms (molecules → atoms) you need to use the coefficients in the molecular formula. For example, and H_2O molecule contains an atom of O and two atoms of H, and hence the relation between water molecules and H and O atoms is:

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

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:

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

Sample Problem 32

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; (c) The number of O atoms in 4.5 moles of NO₂.

SOLUTION

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

$$\begin{aligned} 3.4 \text{ moles of CuO} &\times \frac{6.022 \times 10^{23} \text{ molecules of CuO}}{1 \text{ mole of CuO}} = \\ &= 2.05 \times 10^{22} \text{ molecules of CuO} \end{aligned}$$

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

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

(c) 4.5 moles of NO₂ contains 5.4×10^{24} O atoms, as

$$\begin{aligned} 4.5 \text{ moles of NO}_2 &\times \frac{6.022 \times 10^{23} \text{ NO}_2 \text{ molecules}}{1 \text{ mole of NO}_2} \times \frac{2 \text{ O atoms}}{1 \text{ NO}_2 \text{ molecule}} \\ &= 5.4 \times 10^{24} \text{ O atoms} \end{aligned}$$

◆ STUDY CHECK

The chemical formula for caffeine is C₈H₁₀N₄O₂. Calculate the number of C, H, N and O atoms in 3.5 moles of caffeine.

Answer: 3.4×10^{25} moles of C, 4.2×10^{25} moles of H, 1.7×10^{25} moles of N and 8.4×10^{24} moles of O.

▼The molecular mass of cinnamic acid (C₉H₈O₂), used in the manufacture of flavors, is $148.16 \frac{\text{g}}{\text{mol}}$



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▼Car batteries contain sulfuric acid (H₂SO₄), a corrosive chemical with a molar mass of $180.06 \frac{\text{g}}{\text{mol}}$



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▼Ammonia smelling salts ((NH₄)₂CO₃, 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 weight 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 weight a mole of water (H₂O) we will be weighting 18 grams of water, or if you weight 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).

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Figure 4.2: Examples of measuring equipment

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, H₂O 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 . In order 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 C₂H₄O₂ that 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(NO₃)₂ contains 1Ca, 2N, and 6O, and its molar mass is 164.09g/mol.

730

Sample Problem 33

Calculate: (a) The atomic weight of Mg; (b) the molecular mass of sulfuric acid, H₂SO₄

SOLUTION

(a) According to the periodic table the atomic weight (AW) of Mg is 24.31g/mol. (b) The molar mass of H₂SO₄ 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 C₆H₁₂O₆

Answer: 180.06g/mol.

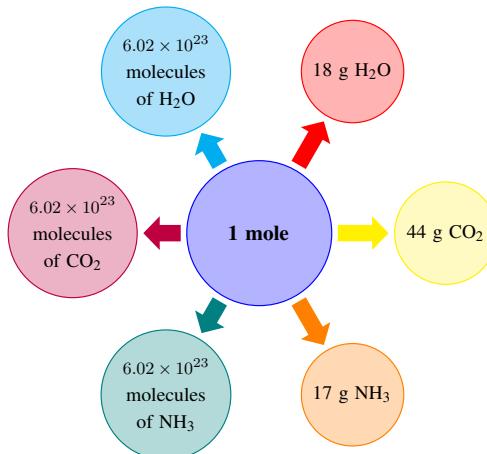
From moles to grams The molar mass is used to convert moles to grams or grams to mol. For example, the molar mass of water is 18g/mol. This means:

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

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 4.3: A mole is equivalent to the same number of molecules for different chemicals. Differently, a mole is equivalent to different weights of different chemicals.



Sample Problem 34

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: $2 \times 5 + 8 \times 1 + 1 \times 12 + 3 \times 16 = 96 \text{ g/mol}$. In order to calculate the moles given the gram, you need to use the molar mass as a conversion factor:

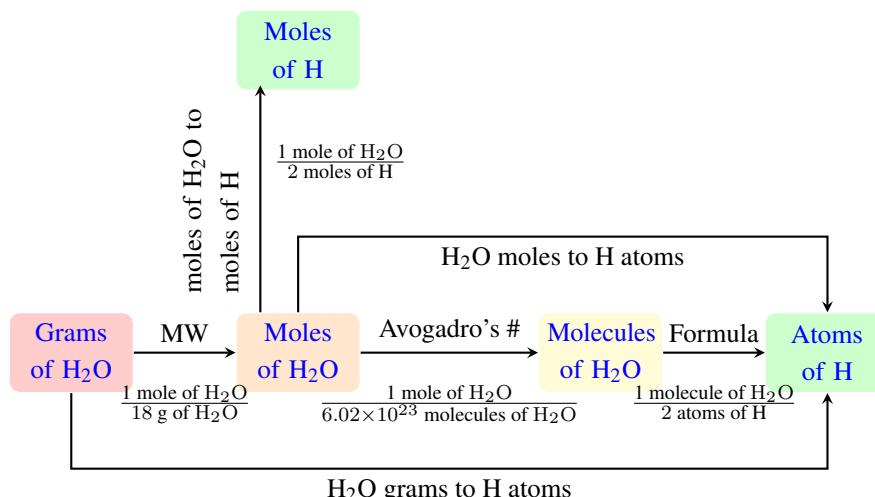
$$100 \text{ g of } (\text{NH}_4)_2\text{CO}_3 \times \frac{\text{moles of } (\text{NH}_4)_2\text{CO}_3}{96 \text{ g of } (\text{NH}_4)_2\text{CO}_3} = 1.04 \text{ moles of } (\text{NH}_4)_2\text{CO}_3$$

◆ STUDY CHECK

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

Answer: 58.4 g/mol; 1168g.

From grams to atoms In the previous sections we covered how to convert grams to moles, and moles to molecules, or molecules to atoms. You can follow the diagram below in order 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.

Sample Problem 35

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: $\text{Fe}_2\text{O}_3 + 2\text{Al} \longrightarrow 2\text{Fe} + \text{Al}_2\text{O}_3$



© www.wallpaperflare.com

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



© www.wallpaperflare.com

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



750

© wikipedia

▼ Wood burning is a combustion reaction



760

© PngImg

Figure 4.4: Examples of reactions

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.

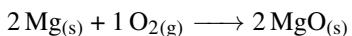
Answer: 332.1g.

745

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 basic of chemical reactions. You will learn how to balance reaction and how classify reactions.

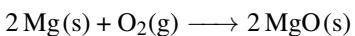
Simple chemical reactions Magnesium is a metal that react with oxygen to produce magnesium oxide. Magnesium is solid $\text{Mg}_{(s)}$ whereas oxygen is gas and contains two oxygen atoms per molecule $\text{O}_{2(g)}$. Magnesium oxide, the result of the reaction, is solid $\text{MgO}_{(s)}$. The reaction between magnesium and oxygen to produce magnesium oxide



Mg and O_2 combine together—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 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 Chemicals reactions can be read in words. In order 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

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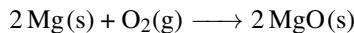
should be read as: “two moles of Mg react with one mole of O_2 to produce two moles of MgO ”.

Balanced chemical reactions Chemical reactions contain molecules, which are made of atoms. Some chemical reactions are balanced, and others need to be

775 balanced. In order 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.

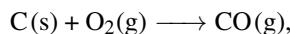


Reactants	Products
2Mg	2Mg ✓
O ₂ =2O	2O ✓

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

785

Now consider the following reaction:



The number of C atoms in the reactants and products is the same, and equals to 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*.

790

Reactants	Products
1C	1C ✓
O ₂ =2O	O ✗

Balancing chemical reactions In order to balance a reaction, we need to introduce the stoichiometric coefficients that make the number of atoms of reactants and products the same. In order 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:

795

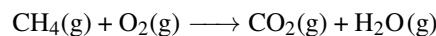
$2 \text{C(s)} + \text{O}_2\text{(g)} \longrightarrow 2 \text{CO(g)}$		
Reactants	Products	
2C	2C ✓	
O ₂ =2O	2O ✓	

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.

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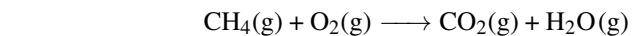
Sample Problem 36

Balance the following reaction:



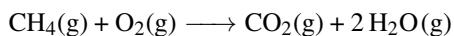
SOLUTION

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:



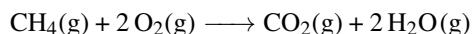
Reactants	Products	
1C	1C	✓
4H	2H	✗
2O	3O	✗

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	✓

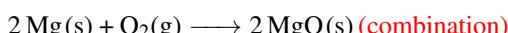
◆ STUDY CHECK

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

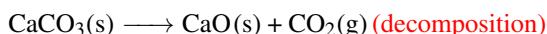
Answer: $\text{Fe}_2\text{O}_3(\text{s}) + 3 \text{C}(\text{s}) \longrightarrow 2 \text{Fe}(\text{s}) + 3 \text{CO}(\text{g})$.

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

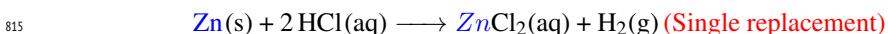
805 In a *combination reaction* two reactants combine to generate a product. An example of a combination is the reaction between Mg and oxygen to produce MgO:



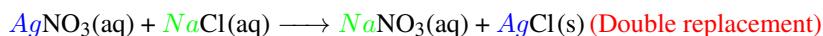
810 In a *decomposition reaction* a single reactant breaks down into several products. An example of a decomposition reaction is the thermal reaction of CaCO_3 to produce calcium oxide (CaO) and carbon dioxide



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 switch places. An example is the reaction between AgNO_3 and NaCl , in which Ag from AgNO_3 replaces Na in NaCl :

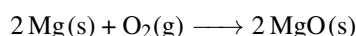


820 Finally, in a combustion reaction, a carbon-based chemical reacts with oxygen to produce carbon dioxide and water. An example would be the combustion of methane (CH_4):



4.4 Stoichiometry and mass calculations

In the previous section, you learned how to balance a chemical reaction. In order 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:

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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 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 product.

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

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

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 do we need to react with Mg, we will proceed as:

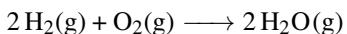
$$5 \frac{\text{moles of Mg}}{} \times \frac{1 \text{ mole of O}_2}{2 \text{ moles of Mg}} = 2.5 \text{ moles of O}_2.$$

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

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Sample Problem 37

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 H_2 ; (b) the number of moles of oxygen needed to react with 7 moles of H_2 .

SOLUTION

(a) we will first convert 5 moles of H_2 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 O_2 will react with 7 moles of H_2 .

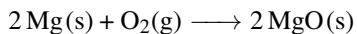
 **STUDY CHECK**

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

Answer: 8 moles.

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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 based the following examples in the reaction of Mg and O_2 :



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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 H_2O is 18 g/mol . If we need to convert 12 grams of water into mols we should do:

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

845

In order 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 in order to operate with them you can only use moles.

Grams to moles in a reaction 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:

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

Now we aim to calculate the number of MgO moles produced from 5 grams of Mg ($\text{AW}=24 \text{ g/mol}$). This times, we will have first to convert the grams of Mg into moles

to then use the mole ration between Mg and MgO:

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

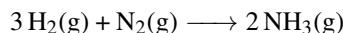
Grams to grams in a reaction We want to answer the following question: we have 6 moles of Mg (AW=24g/mol) and we want to calculate the mass of MgO(MW=40g/mol) produced. The importance of this type of calculations is based on the fact that in a chemistry laboratory chemicals are normally weighted in grams. In order 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:

$$\begin{aligned} 5 \text{ grams of Mg} &\times \frac{1 \text{ moles of Mg}}{24 \text{ grams of Mg}} \times \frac{2 \text{ moles of MgO}}{2 \text{ moles of Mg}} \times \frac{40 \text{ grams of MgO}}{1 \text{ moles of MgO}} \\ &= 10 \text{ grams of MgO}. \end{aligned}$$

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

Sample Problem 38

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:

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

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:

$$\begin{aligned} 10 \text{ grams of N}_2 &\times \frac{1 \text{ moles of N}_2}{28 \text{ grams of N}_2} \times \frac{2 \text{ moles of NH}_3}{1 \text{ moles of N}_2} \times \frac{17 \text{ grams of NH}_3}{1 \text{ moles of NH}_3} \\ &= 12.14 \text{ grams of NH}_3. \end{aligned}$$

❖ STUDY CHECK

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

Answer: 14 grams.

4.5 Percent yield and limiting reagent

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, the 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) reagent.

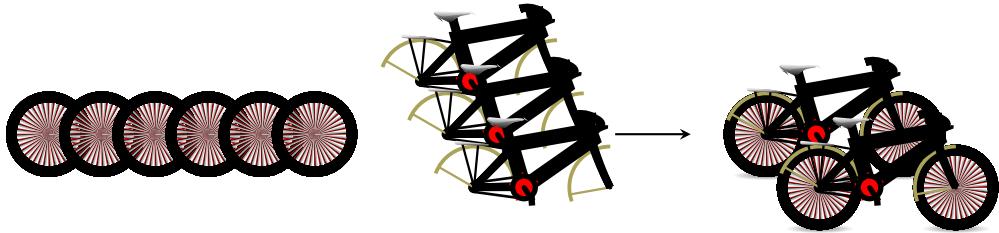
Percent yield Chemical reactions are less than perfect as starting material does not fully convert into products. Furthermore, side reactions often occur in competition with the main reaction generating byproducts. The theoretical yield is the amount of products one will expect in a hypothetically perfect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

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

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.

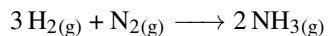


If we have three pairs of wheels and three bodies and we only produce two bikes, the yield will be 67%.



Sample Problem 39

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 produced from 4 moles of hydrogen:

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

Hence the theoretical yield is 2.66 moles of NH_3 , and the actual yield given in the problem is 2 moles of NH_3 . 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:

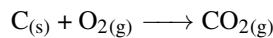
$$\text{Percent Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100 = \frac{2}{2.66} \times 100 = 75.18\%$$

◆ STUDY CHECK

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

Answer: 75%.

⁸⁷⁵ *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 the limiting reactant.

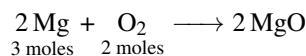
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Often times a reaction will be accompanied with the reagent quantities and you will have to identify the limiting reagent. This reagent will limit the amount of product formed, and hence, any stoichiometric calculation aimed to predict the amount of 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.

890

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



In order to identify the limiting reagent, we will chose 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:

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

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,

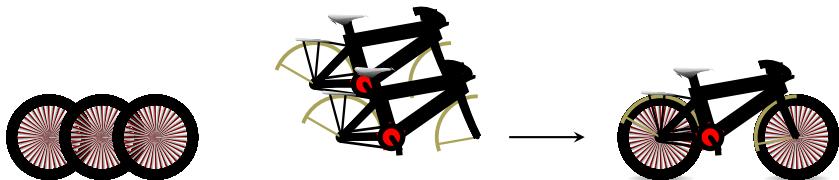
$$n_{\text{needed}}^{\text{O}_2} < n_{\text{given}}^{\text{O}_2}$$

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

$$n_{left}^{O_2} = |n_{needed}^{O_2} - n_{given}^{O_2}| = 0.5 \text{ moles of O}_2$$

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

895

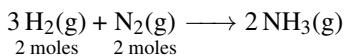


Differently, if we have three wheels and one body, then the body of the bikes limit the production.



Sample Problem 40

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:

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

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

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.

Answer: N_2 is the limiting reagent and H_2 the excess. 0.5 moles of hydrogen will remain.

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:

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

4.7 Fill the conversion factor that calculates the final property:

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

4.8 Fill the conversion factor that calculates the final property:

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

ATOMS

4.9 Calculate the molar weight of the following molecules: (a) NH₃ (b) O₂ (c) CO (d) H₂ (e) Fe₂(CO₃)₃

4.10 Fill the conversion factor that calculates the final property:

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

4.11 Fill the conversion factor that calculates the final property:

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

4.12 Fill the conversion factor that calculates the final property:

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

4.13 Fill the conversion factor that calculates the final property:

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

4.14 Fill the conversion factor that calculates the final property:

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

4.15 Fill the conversion factor that calculates the final property:

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

4.16 Fill the conversion factor that calculates the final property:

$$\frac{6 \text{ molecules of } C_6H_{12}O_6}{\text{_____}} \times \frac{\text{_____}}{\text{_____}} \\ = \text{_____ atoms of C.}$$

4.17 Fill the conversion factor that calculates the final property:

$$\frac{10^{21} \text{ atoms of N}}{\text{_____}} \times \frac{\text{_____}}{\text{_____}} \\ = \text{_____ molecules of } CH_4N_2O.$$

4.18 Answer the following questions: (a) Calculate the number of C atoms in 3 moles of $C_{10}H_{14}N_2$? (b) Calculate the number of H atoms in 3 moles of $C_{10}H_{14}N_2$? (c) Calculate the number of N atoms in 3 moles of $C_{10}H_{14}N_2$

4.19 Answer the following questions: (a) How many grams are there in 4 moles of $C_6H_{12}O_6$? (b) How many C atoms are there in 3 moles of $C_6H_{12}O_6$? (c) How many O atoms are there in 3 moles of $C_6H_{12}O_6$?

CHEMICAL REACTIONS

4.20 Balance the following reactions:

- (a) $P_4(s) + O_2(g) \longrightarrow P_4O_{10}(s)$
 (b) $Al(s) + O_2(g) \longrightarrow Al_2O_3(s)$

4.21 Balance the following reactions:

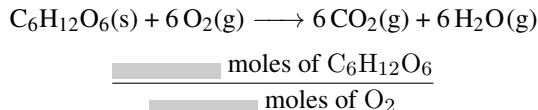
- (a) $FeS(s) + O_2(g) \longrightarrow Fe_2O_3(s) + SO_2(g)$
 (b) $NH_3(g) + O_2(g) \longrightarrow NO(g) + H_2O(g)$

4.22 Classify next reaction as combination, decomposition, single replacement, double replacement, or combustion:

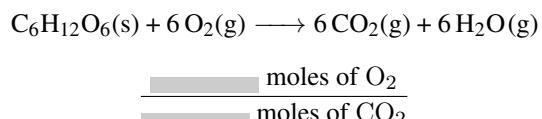
- (a) $Pb_{(s)} + FeSO_{4(s)} \longrightarrow PbSO_{4(s)} + Fe_{(s)}$
 (b) $C_6H_{12(g)} + 9 O_{2(g)} \longrightarrow 6 CO_{2(g)} + 6 H_2O_{(g)}$
 (c) $2 RbNO_{3(aq)} + BeF_{2(aq)} \longrightarrow Be(NO_3)_{2(aq)} + 2 RbF_{(aq)}$

STOICHIOMETRY AND MASS CALCULATIONS

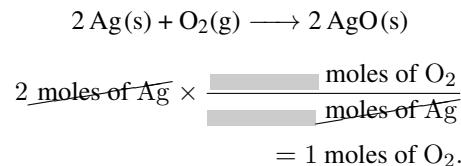
4.23 Fill the mole ratio for the following reaction:



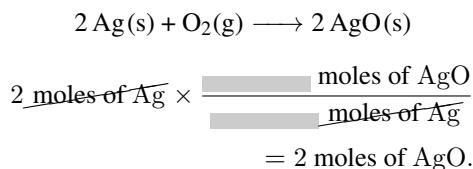
4.24 Fill the mole ratio for the following reaction:



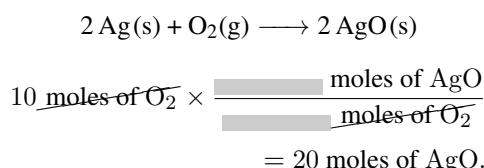
4.25 Fill the conversion factor that calculates the moles of oxygen needed to react with 2 moles of Silver producing AgO :



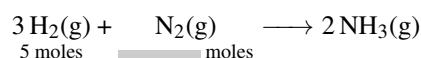
4.26 Fill the conversion factor that calculates the moles of AgO produced from 2 moles of Silver:



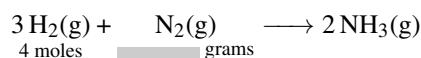
4.27 Fill the conversion factor that calculates the moles of AgO produced from 10 moles of oxygen:



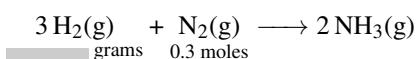
4.28 Calculate how many moles of nitrogen are needed to react with 5 moles of hydrogen, to produce ammonia:



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

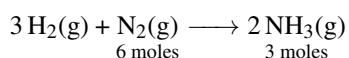


4.30 Calculate the number of grams of hydrogen needed to react with 0.3 moles of nitrogen, to produce ammonia:

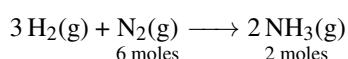


PERCENT YIELD AND LIMITING REAGENT

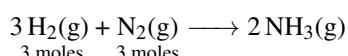
4.31 Six moles of nitrogen gas react to produce three moles of ammonia according to the following reaction:



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

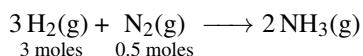


4.33 We mix three moles of hydrogen gas with three moles of nitrogen gas.



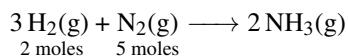
Calculate the limiting reagent.

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



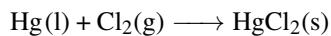
Calculate the limiting reagent.

4.35 We mix two moles of hydrogen gas with five moles of nitrogen gas.



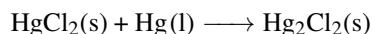
Calculate the limiting reagent.

4.36 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 HgCl_2 . What is the percent yield of the reaction.

4.37 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.

4.38 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%.

4.39 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).

GENERAL PROBLEMS

4.40 Calculate the molar weight of the following molecules: (a) benzene, C_6H_6 (b) Carbon disulfide, CS_2 (c) Nitrogen tetroxide, N_2O_4

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

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

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

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

$$\begin{aligned} 5 \times 10^{25} \text{ atoms of H} &\times \frac{\text{_____}}{\text{_____}} \times \frac{\text{_____}}{\text{_____}} \\ &\times \frac{\text{_____}}{\text{_____}} = \text{_____ g of C}_2\text{H}_6 \end{aligned}$$

4.44 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)

- Answers**
- 4.1** (a) 4.8×10^{24} (b) 6.0×10^{24} **4.3** (a) 0.99 moles of NO (b) 8.3×10^{-9} moles of NaCl
 (c) 4983.39 moles of MgO **4.5** 10^{24} molecules of $\text{NO}_2 \times \frac{1 \text{ moles of } \text{NO}_2}{6.02 \times 10^{23} \text{ molecules of } \text{NO}_2} = 1.66 \text{ moles of } \text{NO}_2$.
- 4.7** $6 \text{ moles of } \text{C}_6\text{H}_{12}\text{O}_6 \times \frac{6.02 \times 10^{23} \text{ molecules of } \text{C}_6\text{H}_{12}\text{O}_6}{1 \text{ mole of } \text{C}_6\text{H}_{12}\text{O}_6} = 3.6 \times 10^{24} \text{ molecules of } \text{C}_6\text{H}_{12}\text{O}_6$. **4.9** (a) 17
 $\text{g} \cdot \text{mol}^{-1}$ (b) $32 \text{ g} \cdot \text{mol}^{-1}$ (c) $28 \text{ g} \cdot \text{mol}^{-1}$ (d) $2 \text{ g} \cdot \text{mol}^{-1}$ (e) $218 \text{ g} \cdot \text{mol}^{-1}$ **4.11** $10 \text{ g of NO} \times \frac{1 \text{ moles of NO}}{30 \text{ g of NO}} = 0.33 \text{ moles of NO}$. **4.13** $7 \text{ g of } \text{CH}_4\text{N}_2\text{O} \times \frac{1 \text{ mol of } \text{CH}_4\text{N}_2\text{O}}{60 \text{ g of } \text{CH}_4\text{N}_2\text{O}} = 0.12 \text{ moles of } \text{CH}_4\text{N}_2\text{O}$. **4.15** $10^{22} \text{ atoms of O} \times \frac{1 \text{ molecules of H}_2\text{O}}{2 \text{ atoms of O}} = 5 \times 10^{21} \text{ molecules of H}_2\text{O}$ **4.17** $10^{21} \text{ atoms of N} \times \frac{1 \text{ molecules of } \text{CH}_4\text{N}_2\text{O}}{1 \text{ atoms of N}} = 10^{21} \text{ molecules of } \text{CH}_4\text{N}_2\text{O}$ **4.19** (a) 720.64 grams (b) 2×10^{27} atoms (c) 3.9×10^{27} atoms **4.21** (a) $4 \text{ FeS(s)} + 7 \text{ O}_2(\text{g}) \longrightarrow 2 \text{ Fe}_2\text{O}_3(\text{s}) + 4 \text{ SO}_2(\text{g})$ (b) $4 \text{ NH}_3(\text{g}) + 5 \text{ O}_2(\text{g}) \longrightarrow 4 \text{ NO(g)} + 6 \text{ H}_2\text{O(g)}$ **4.23** 1/6 **4.25** 1/2 **4.27** 20
4.29 37.3 g **4.31** 25% **4.33** H_2 **4.35** H_2

PART D

5

Reactions in solution

THE most common reactions happen in solution. Think, for example, when you add sugar to your coffee or how a metal rusts when it gets wet. The first example involves a dissociation reaction, whereas the second a redox reaction.

This chapter first covers the properties of solutions and the quantification of the amount of solute in a solution. This chapter also covers some important types of reactions happening in solution. Another important concept covered in this chapter is the idea of electrolytes. On one hand, most of you will be surprised to know that water do not conduct the 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 sport drink. These are actually electrolyte solutions. However, few know the specifics of their function. Electrolytes are actually salts that conduct electricity in water by separating into positive and negative ions. In this chapter, you will be able to identify different types of electrolytes. Finally, here we will also cover some important reactions happening in solution. In particular reactions between acids and base, reaction that result in a solid and reaction involving an electron exchange.



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GOALS

910

- 1 Carry composition calculations
- 2 Classify electrolytes
- 3 Identify insoluble compounds
- 4 Write down net ionic equations
- 5 Balance redox reactions

915

Discussion: List three solutions in your household containing just a single solute. Give the chemical formula of the solute and the name of the solvent.

920

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 affect the formation of a solution. For example, a solution will not result from mixing oil and water as they have different polar character 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.

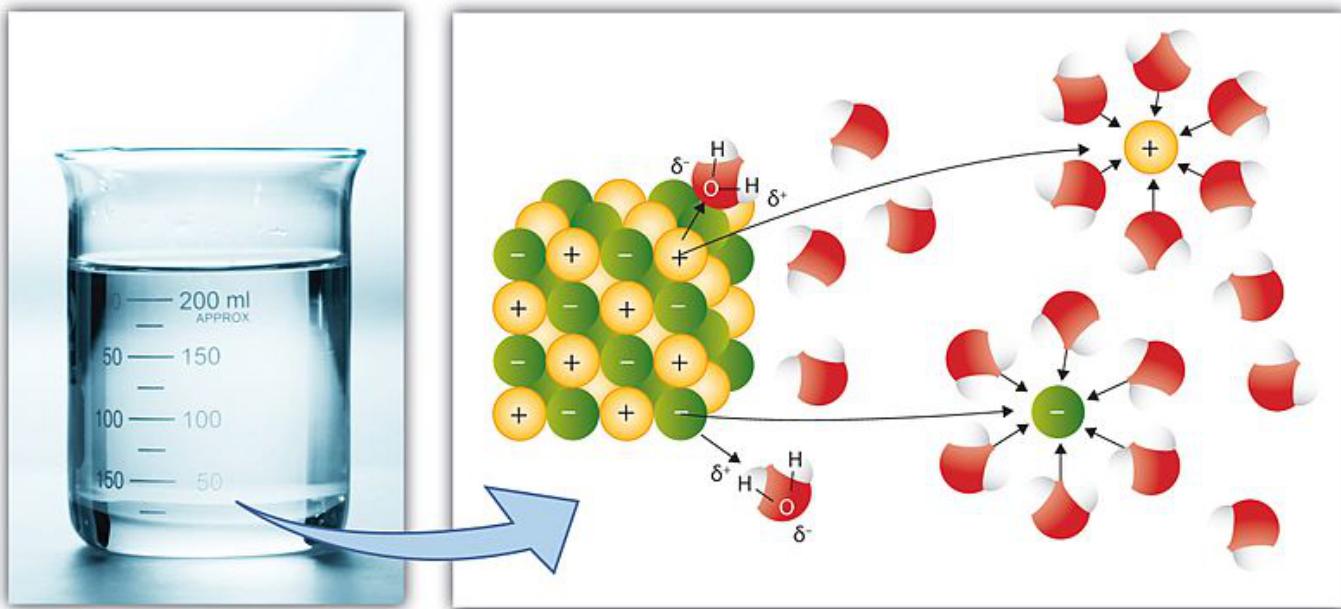
What makes a solution? Solutions are homogeneous mixtures of a solute and a solvent. Homogeneous means that if you look at the mixture you will not be able to differentiate both components and you will only see it as a whole. In a solution, the solute is the component of the mixture in less amount, whereas 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 the result of mixing a solute and a solvent:

$$\text{Solution} = \text{Solute} + \text{Solvent}$$

Types of solutions You can prepare different types of solutions by mixing a solid

925

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.



© Wikipedia

Figure 5.1: A solution results from dissolving a solute into a solvent

930 *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 H_2 molecule. Differently, HF is a polar molecule, as F concentrates more 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 together creating a single visible phase. As an example, water (H_2O , polar) and methanol (CH_3OH , polar) will mix together. Differently, water (polar) and oil (non-polar) are immiscible due to its different polar nature and they will not mix. Even if the rules of 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:

- 935
- Diatomic molecules made of the same element (e.g. H_2) are non-polar.
 - Diatomic molecules made of different elements (e.g. HI) are polar.
 - Poliatomic molecules (with more than four atoms) made of C and H (e.g. CH_4) are in general non-polar.
 - Poliatomic molecules (with more than four atoms) containing C, H and a different atom (e.g. CH_3F) are in general polar.

Sample Problem 41

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.

Answer: polar, nonpolar, nonpolar, polar.

950

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) 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). 955

Sample Problem 42

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)}

Answer: (a) will mix; (b) will not mix.

Concentration of solutions One of the most important properties of a solution is its concentration. The larger the concentration of a solution the more solute in the solution. There are many different concentration units, such as molarity or mass percent concentration. This section will introduce you to some of the most important concentration units. 960

Meaning of concentration The concentration of a solution refers to the amount of solute with respect to the amount of solution. The larger concentration the larger number of solute particles with respect to the solution. 965

Mass percent concentration The mass percent (m/m) is the amount of solute in grams per grams of solution in percent form

$$m/m = \frac{\text{g of solute}}{\text{g of solution}} \times 100$$

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 43

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: 52mL = $5.2 \times 10^{-2} \text{ L}$. 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 KCl 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 5g of KCl with 200g of H₂O. Calculate the percent (m/m) of the solution.

Answer: 0.43M; 2.4 %.

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 is 3 moles of solute every one litter of solution.

$$3M \quad \text{or} \quad \frac{3 \text{ mol of solute}}{1 \text{ L of solution}} \quad \text{or} \quad \frac{1 \text{ L of solution}}{3 \text{ mol of solute}}$$

Similarly, if the mass percent of a solution is 5% this means that there is 5 grams of solute every 100 grams of solution. We often use concentration units as conversion factors when we need to transform between on unit on top (bottom) of the conversion factor and the unit on the bottom (top).

Sample Problem 44

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.

Answer: 83.3g.

Dilution Dilution is the process for preparing a diluted solution from a more concentrated solution. Solutions are often times stored in a stock room in concentrated form. These stocks should be diluted before use. In order 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. In order to answer this we should use the following formula:

$$c_1 \cdot V_1 = c_2 \cdot V_2$$

Sample Problem 45

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.

Answer: 1.8 L.

5.2 Electrolytes and insoluble compounds

On one hand, electrolytes are compounds that conduct the electricity once dissolved in water. Differently, nonelectrolytes are compounds that do not conduct the 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.

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? The Table below will help you predict the solubility of a salt. In order to do this, you need to start by assess the right ion (the anion, CrO_4^{2-}) located on the left column of the Table below. After that you need to assess the left ion (the cation, Ba^{2+}) located on 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 46

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

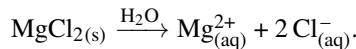
Predict the soluble/insoluble nature of the following compounds: (a) Li_3PO_4 , (b) Na_2S and (c) AgCl .

Answer: (a) $\text{Li}_3\text{PO}_4(aq)$ soluble, (b) $\text{Na}_2\text{S}(aq)$ soluble and (c) $\text{AgCl}(s)$ insoluble.

Table ?? 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^-)	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^+)

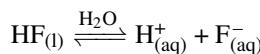
Strong electrolytes Strong electrolytes completely dissociate in water. Hence, in a solution of a strong electrolyte you will only have ions and never molecules. Strong electrolytes are typically ionic compounds such as MgCl₂ or NaCl (table salt). We represent the dissociation of a strong electrolyte with a single arrow, meaning that the reaction proceeds to completion and for the example below, in the solution we will only have ions (Mg²⁺_(aq) + 2 Cl⁻_(aq)) and not molecules (MgCl_{2(s)}):



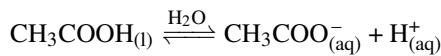
1000

Weak electrolytes Weak electrolytes partially dissociate in water, and this is indicated by means of 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:

1005

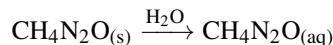


Acetic acid (CH₃COOH) is an important weak electrolyte and its dissociation proceeds somehow in a peculiar way:



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 CH₄N₂O proceeds as:

1010



Identify the electrolyte character of a chemical You can use the Table below to identify the electrolyte character of a chemical. Ionic compounds are in general strong electrolytes, and most acids 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. C₁₂H₂₂O₁₁) are in general nonelectrolytes.

1015

1020

Sample Problem 47

For the following chemicals indicate whether you will have in the solution (a) only ions, (b) ions and some molecules, or (c) molecules: NH₃, KOH, and C₁₂H₂₂O₁₁.

SOLUTION

Ammonia (NH₃) 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 (C₁₂H₂₂O₁₁) is a nonelectrolyte and in solution you will find molecules.

◆ STUDY CHECK

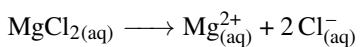
For the following chemicals indicate whether you will have in the solution only ions, ions and some molecules, or molecules: (a) H₂SO₄, HNO₃ and CH₃OH.

Answer: (a) ions, (b) ions (c) molecules.

Table ?? 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 ₂ SO ₄ , etc
Weak	Partially	Ions & molecules	NH ₃ , CH ₃ COOH (acetic acid), HF, H ₂ O
Nonelectrolytes	No	molecules	Most covalent compounds: CH ₃ OH (methanol), CH ₃ CH ₂ OH (ethanol), C ₁₂ H ₂₂ O ₁₁ (sucrose), CH ₄ NO ₂ (urea)

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 Na⁺_(aq) cations and Cl⁻_(aq) anions. Hence it is important to correctly break down electrolytes into ions. In order 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 MgCl₂ formula also tells us we have one magnesium and two chlorines. The overall process is:



Another example, magnesium nitrate Mg(NO₃)₂. This strong electrolyte—as this is an ionic salt—is made of lithium with valence +I and nitrate with valence -I. The formula indicates we have one Mg²⁺_(aq) and two NO₃⁻_(aq). Hence:



Sample Problem 48

Break down the following chemicals into ions, if possible:

Chemical	Particles in solution
K ₂ CrO _{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, K₂CrO_{4(aq)} is named potassium chromate and contains 2K⁺_(aq) and CrO₄²⁻_(aq) ions. Barium nitrate—Ba(NO₃)_{2(aq)}—will produce Ba²⁺_(aq) and 2NO₃⁻_(aq). Finally, potassium nitrate—KNO_{3(aq)}—will produce K⁺_(aq) and NO₃⁻_(aq). In the table:

Chemical	Particles in solution
$\text{K}_2\text{CrO}_4(\text{aq})$	$2\text{K}_{(\text{aq})}^+ + \text{CrO}_4^{2-}(\text{aq})$
$\text{Ba}(\text{NO}_3)_2(\text{aq})$	$\text{Ba}_{(\text{aq})}^{2+} + 2\text{NO}_3^-(\text{aq})$
$\text{BaCrO}_4(\text{s})$	$\text{BaCrO}_4(\text{s})$
$\text{KNO}_3(\text{aq})$	$\text{K}_{(\text{aq})}^+ + \text{NO}_3^-(\text{aq})$

◆ STUDY CHECK

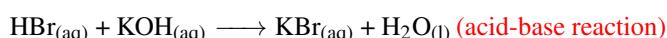
Break down the following chemicals into ions, if possible: $\text{H}_2\text{O}_{(\text{l})}$, $\text{NH}_3_{(\text{l})}$, $\text{AgNO}_3(\text{aq})$.

Answer: $\text{H}_2\text{O}_{(\text{l})}$, $\text{NH}_3_{(\text{l})}$, $\text{Ag}_{(\text{aq})}^+$, $\text{NO}_3^-(\text{aq})$.

5.3 An introduction to reactions in solution

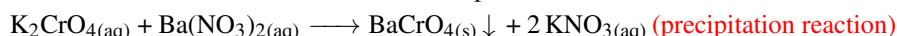
There are three different reactions in solution: acid-base reactions, precipitation reaction and redox reactions. The key to identify acid-base reactions is in the reactants, as an acid-base reaction results from the reaction between an acid and a base. Precipitation reactions are reactions that produce a precipitate. Hence, the key to identify a precipitation reaction is in the products. Precipitation reactions always contain a solid as a product. Redox reactions contain two elements with different redox number in the reactants and products. The key to identify redox reactions is to be able to spot elements with different oxidation state, for example: Cu and Cu^{2+} or H^+ and H_2 . 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 they produce water and another chemical. An example is:



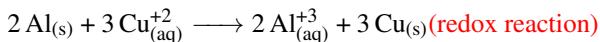
Hydrobromic acid (HBr) is an acid and potassium hydroxide (KOH) a base. The result of an acid-base reaction is always water and an ionic compound, in this case KBr .

Precipitation reactions Precipitation reactions result in an insoluble chemical, that is, results in a solid chemical. An example would be:



The chemical $\text{BaCrO}_4(\text{s})$ is a solid that precipitates in the solution, hence the name of the type of reaction. The symbol on $\text{BaCrO}_4(\text{s}) \downarrow$ represents the precipitation process. The solubility of a given solute such as $\text{BaCrO}_4(\text{s})$ is the amount of solute (in grams) that can be dissolve 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 reaction are different than acid-base or precipitation reaction. They contain the same chemical element in two different states resulting from the loss or win of electrons. Look for example:



We have that neither $\text{Al}_{(\text{s})}$ or $\text{Cu}_{(\text{aq})}^{+2}$ 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 $\text{Al}_{(\text{s})}$ and as ionic $\text{Al}_{(\text{aq})}^{+3}$, which result from the loss of three electron. Therefore in redox reaction there is always elements in the chemicals that lose electrons. In redox reactions there is also an element that wins electrons. For example, $\text{Cu}_{(\text{s})}$ and $\text{Cu}_{(\text{aq})}^{+2}$ have different redox number. In particular, $\text{Cu}_{(\text{aq})}^{+2}$ is the result of removing three electrons from $\text{Cu}_{(\text{s})}$. 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 49

Classify the following reactions as acid-base, redox or precipitation.

- (a) $\text{Fe}_{(\text{s})} + \text{Cu}_{(\text{aq})}^{+2} \longrightarrow \text{Fe}_{(\text{aq})}^{+2} + \text{Cu}_{(\text{s})}$
- (b) $\text{AgNO}_3_{(\text{aq})} + \text{NaCl}_{(\text{aq})} \longrightarrow \text{AgCl}_{(\text{s})} + \text{NaNO}_3_{(\text{aq})}$
- (c) $2 \text{HCl}_{(\text{aq})} + \text{Ca(OH)}_2_{(\text{aq})} \longrightarrow \text{CaCl}_2_{(\text{aq})} + 2 \text{H}_2\text{O}_{(\text{l})}$

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.

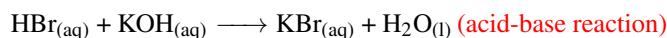
- (a) $\text{HNO}_2_{(\text{aq})} + \text{NaOH}_{(\text{aq})} \longrightarrow \text{NaNO}_2_{(\text{aq})} + \text{H}_2\text{O}_{(\text{l})}$
- (b) $2 \text{Na}_{(\text{s})} + \text{Cl}_2_{(\text{g})} \longrightarrow 2 \text{NaCl}_{(\text{s})}$
- (c) $\text{MgCl}_2_{(\text{aq})} + 2 \text{AgNO}_3_{(\text{aq})} \longrightarrow 2 \text{AgCl}_{(\text{s})} + \text{Mg}(\text{NO}_3)_2_{(\text{aq})}$

Answer: acid-base; redox; precipitation

5.4 Precipitation reactions and acid-base reactions

This section deal 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 other chemical. Precipitation reactions produce a precipitate, that is, a solid.

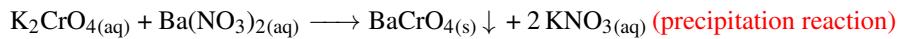
Acid-base reactions Acid-base reactions result from the reaction of an acid with a base. Both they produce water and another chemical. An example is:



Hydrobromic acid $\text{HBr}_{(\text{aq})}$ is an acid and potassium hydroxide a base.

Precipitation reactions Precipitation reactions result in an insoluble chemical. 1095

An example would be:



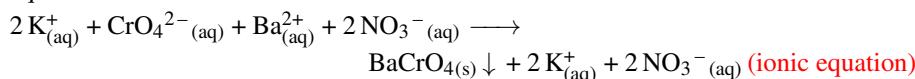
The chemical $\text{BaCrO}_4_{(\text{s})}$ is a solid that precipitates in the solution. The solubility of a given solute such as $\text{BaCrO}_4_{(\text{s})}$ is the amount of solute (in grams) that can be dissolve in a given mass of solvent (in particular 100 g of solvent). A solute with a low solubility 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. 1100 1105

Formula equations, ionic equations and net ionic equations

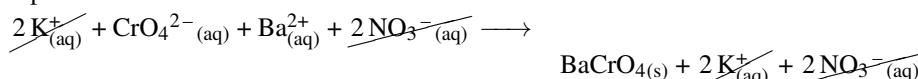
Electrolytes in solutions contains ions—cations and anions—however, when we write chemical formulas we barely show those ions. Differently, we just write the formulas and that is the reason that chemical equations are referred as *formula equation*. Look for example: 1110



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 solution, as it is a solid. Ionic equations result from writing all ions in a formula equation: 1115



However, the ionic equation contains repeated ions. Look for example the previous equation with $2\text{K}^+_{(\text{aq})}$ on the left and on the right of the equation. If we simplify the repeated ions 1120



we obtain what is called as the *net ionic equation*:

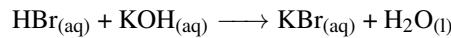


1125

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 in both sides of the equation.

Sample Problem 50

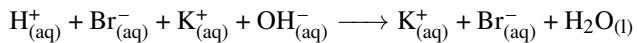
Write down the ionic equation and net ionic for the following formula equation:



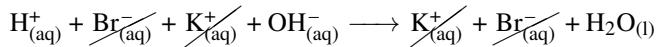
1130

SOLUTION

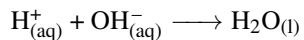
Mind we can only break down strong electrolytes. Hence, water will not be expressed in the form or ions as it is a weak electrolyte. If we break down the other chemicals we have the ionic equation:



If we eliminate the ions that are repeated in both sides:

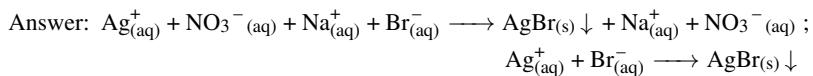
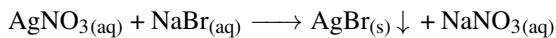


we have the net ionic equation:



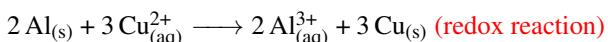
❖ STUDY CHECK

Write down the ionic equation and net ionic for the following formula equation:



5.5 Redox reactions

Redox reaction are different than acid-base or precipitation reaction. 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 charge. 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 smaller this number the more electrons the element has won.

Rules to calculate redox numbers We indicate redox numbers with 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 a non integer number. There is 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.

1155

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. In order 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—equals 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 a redox number of manganese of VII.

Sample Problem 51

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) $\text{Cr}_2\text{O}_7^{2-}$ and (b) Cr_2O_3

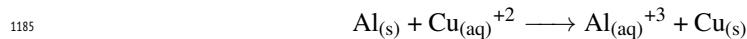
Answer: VI; III.

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 $\text{Cr}^{\text{VI}}_2\text{O}_7^{2-}$ and $\text{Cr}^{\text{III}}_2\text{O}_3$. 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 an element, and that means the element has lost electrons. The smaller the redox number the more reduced is the element and that means it has gained electrons. If we compare both case, we have that Cr in dichromate is oxidized—it lost electrons—and Cr in chromium(III) oxide is reduced—it gained electrons.

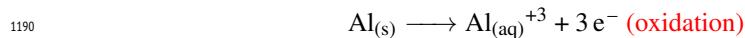
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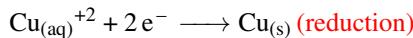
Redox numbers in chemical reactions The goal is to identify the element that undergoes oxidation and reduction in a chemical reaction. We can reach this goal by using the half-reaction method. Every redox reaction is composed of two processes, a reduction and the oxidation. These two processes can be separated into two half-reactions so that the combination of both half-reactions lead to the balanced redox. Let us work on a simple unbalanced redox reaction:



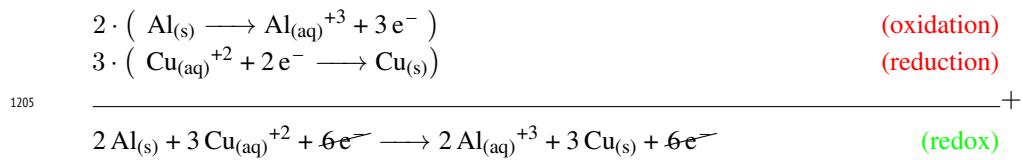
Solid $\text{Al}_{(\text{s})}$ on the reactant side has zero redox number, whereas ionic $\text{Al}_{(\text{aq})}^{+3}$ on the product side has redox number equal to III. Al has undergone oxidation as its redox number increases from zero to three. Al has lost three electrons. We can write the oxidation half-reaction:



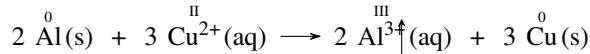
Mind that electrons have negative charge and we add electrons to compensate the charge of $\text{Al}_{(\text{aq})}^{+3}$. Now let us compare the redox number of Cu. In the reactant side we have $\text{Cu}_{(\text{aq})}^{+2}$ with redox of II. In the product side we have $\text{Cu}_{(\text{s})}$ with zero redox number. Cu has undergone reduction as its redox number has decreased. This means it has gained electrons, in particular two electrons:



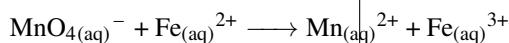
Balancing simple redox reactions The goal here is to balance a redox chemical reaction by combining two half-reactions. In the example above the oxidation and reduction involve different number of electrons. Hence in order to be able to add both redox we need to times each half-reaction by a number so that the number of electrons cancel out. As the first reaction involved three electrons and the second two, we will do:



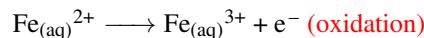
The overall balanced redox equation is:



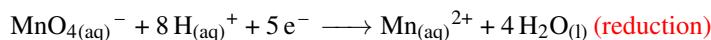
Balancing redox reactions in acidic medium Redox reactions happen in either basic or acidic medium. Here we will go over how to balance redox reactions in acidic medium. In order to do this we will first separate the reaction in two half-reactions. In each semi-reaction we will balance all elements but hydrogen and oxygen. When all elements are balanced, we will proceed to balance O by adding H_2O 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:



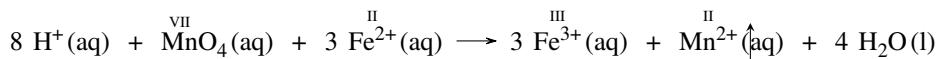
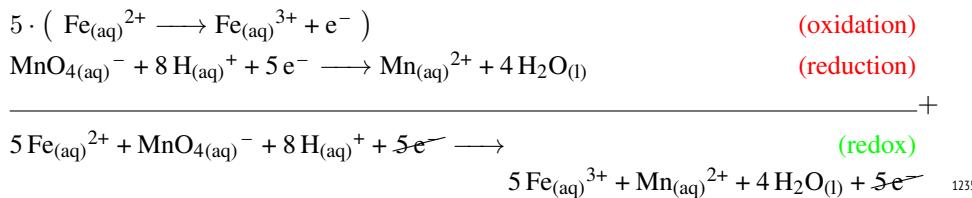
One of the semi-reactions involve Manganese whereas the other involves Iron. The redox number of Mn in permanganate is VII hence Manganese is being reduced, as its redox number decreases from VII to II, whereas Iron is being oxidized as its redox number increases from II to III. The oxidation half-reaction 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 H_2O molecules to balance oxygen and H^+ to balance hydrogen. In particular, we will need two water molecules—as MnO_4^- 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:

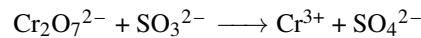


As the oxidation involves one electron and the reduction three, we need to time the oxidation by three:



Sample Problem 52

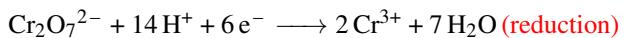
Balance the following redox in acidic medium:



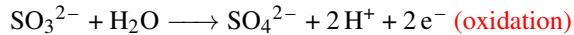
SOLUTION

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:

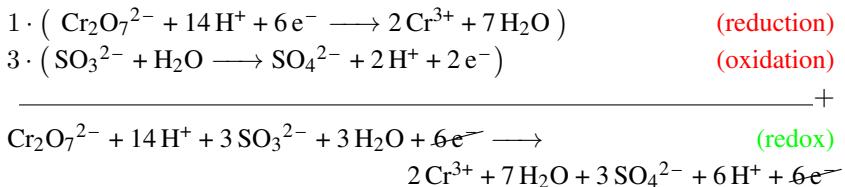
Oxidation: -1e^-



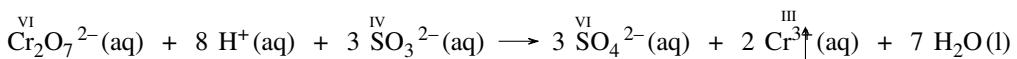
For the reduction half-reaction, we have a difference of one oxygen atoms and hence we will need one water molecule and two protons; we will need two electrons to compensate the charge:



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:

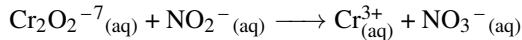


After we cancel the electrons and eliminate protons and water molecules, the balanced reaction is:



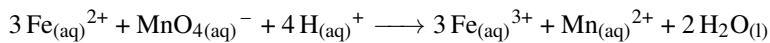
◆ STUDY CHECK

Balance the following redox in acidic medium:

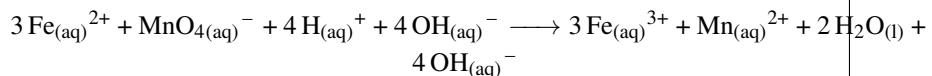


Answer: $3 \text{NO}_2^{-}(\text{aq}) + 8 \text{H}^+(\text{aq}) + \text{Cr}_2\text{O}_2^{-7}(\text{aq}) \longrightarrow 3 \text{NO}_3^{-}(\text{aq}) + 2 \text{Cr}^{3+}_{(\text{aq})} + 4 \text{H}_2\text{O(l)}$.

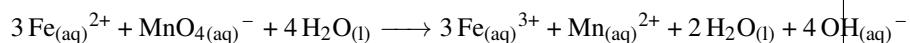
Balancing redox reactions in basic medium In order to balance a redox in basic medium we need first to balance the reaction in acidic medium. After, we will compensate all H^+ with OH^- in both sides of the reaction. Mind that when combining H^+ with OH^- we obtain H_2O . For example, in order to balance the following reaction in basic medium:



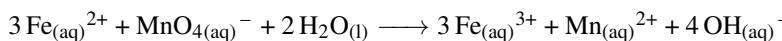
we will add four OH^- in both sides:



And after cancelling 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 $C_6H_{6(l)}$ 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 Which chemicals from the following list will mix with $H_2O_{(l)}$: (a) $NH_3_{(l)}$ (b) $C_5H_{12(l)}$ (c) $C_6H_{14(l)}$

5.4 Which chemicals from the following list will mix with $C_5H_{12(l)}$: (a) $H_2O_{(l)}$ (b) $C_6H_{14(l)}$ (c) $CH_3COOH_{(l)}$

5.5 Classify the following molecules as polar or non-polar: (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) $C_6H_5NH_2_{(l)}$

5.6 Classify the following molecules as polar or nonpolar: (a) $H_2O_{(l)}$ (b) $C_5H_{12(l)}$ (c) $CH_3COOH_{(l)}$ (d) $CH_3OH_{(l)}$

5.7 Oil and water do not mix due to a polarity difference. Explain why a detergent can help solve oil in water.

CONCENTRATION UNITS

5.8 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.

5.9 A solution is prepared by mixing 15g of KCl in 50g of water. Calculate the mass percent of solute.

5.10 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.

5.11 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.

5.12 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.

5.13 How many mL of a 3M KCl solution contains 0.06 moles of KCl .

5.14 How many mL of a 4M $NaCl$ ($MW=58\text{g/mol}$) solution contains 5 grams of $NaCl$.

5.15 How many grams of solute are there in 100mL of a 0.01M HNO_3 ($MW=63\text{g/mol}$) solution.

5.16 How many mL of a 0.001M $Ca(OH)_2$ ($MW=74\text{g/mol}$) solution can be prepared from 5 mg of $Ca(OH)_2$.

5.17 What is the final volume when 50mL of a 2M $NaCl$ solution is diluted to a 1M.

5.18 What is the concentration of a solution prepared when 100mL a 4% HCl solution is diluted to a final volume of 500mL.

5.19 Describe how to prepare 50mL of a 0.5M H_2SO_4 solution, starting with a 1M stock H_2SO_4 solution.

ELECTROLYTES AND INSOLUBLE COMPOUNDS

5.20 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			
$CaCl_2$			
H_2O			
NO_2			

5.21 Indicate the soluble/insoluble character of the following compounds:

Chemical	Soluble	Insoluble
AgNO_3		
AgBr		
CaCO_3		
Na_2CO_3		

5.22 Indicate the soluble/insoluble character of the following compounds:

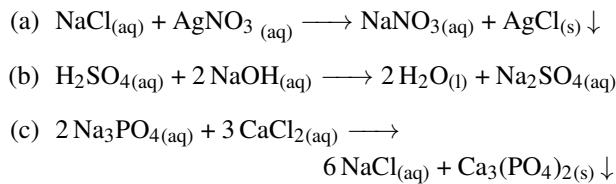
Chemical	Soluble	Insoluble
NaCH_3COO		
NaHCO_3		
Ag_2SO_4		
NaCrO_4		
CaS		

5.23 Break down the following compounds into ions:

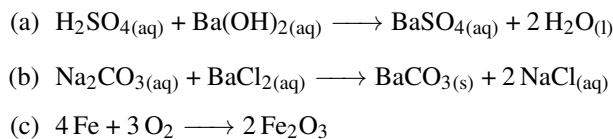
- $\text{Ca}(\text{OH})_2$
- K_2CrO_4
- $\text{Ca}(\text{NO}_3)_2$

PRECIPITATION AND ACID-BASE REACTIONS

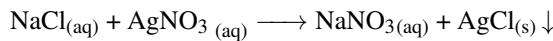
5.24 Classify the following reaction as acid-base or precipitation:



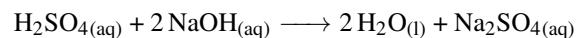
5.25 Classify the following reaction as acid-base or precipitation:



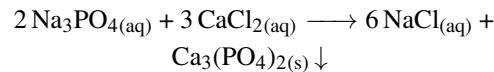
5.26 Obtain the net ionic equation for the following reaction:



5.27 Obtain the net ionic equation for the following reaction:



5.28 Obtain the net ionic equation for the following reaction:



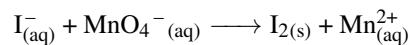
REDOX

5.29 Balance the following redox reactions:

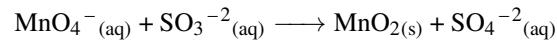
- $$(a) \text{ Fe}_{(s)} + \text{O}_{2(g)} \longrightarrow \text{Fe}_{(aq)}^{3+} + \text{O}_{(aq)}^{2-}$$

$$(b) \text{ Cu}_{(s)} + \text{Ag}_{(aq)}^+ \longrightarrow \text{Ag}_{(s)} + \text{Cu}_{(aq)}^{2+}$$

5.30 Balance the following redox reactions in acidic medium:



5.31 Balance the following redox reactions in acidic medium:



5.32 Balance the following redox reactions in acidic medium:

- $$(a) \text{Zn}_{(s)} + \text{NO}_3^-_{(\text{aq})} \longrightarrow \text{Zn}_{(\text{aq})}^{2+} + \text{NO}_2_{(\text{g})}$$

$$(b) \text{O}_2_{(\text{g})} + \text{Fe}_{(\text{aq})}^{2+} \longrightarrow \text{Fe}_{(\text{aq})}^{3+}$$

5.33 Balance the following redox reactions in basic medium:

- (a) $\text{Sn}_{(\text{aq})}^{2+} + \text{Cr}_2\text{O}_7^{2-} \rightarrow \text{Cr}_{(\text{aq})}^{3+} + \text{Sn}_{(\text{aq})}^{4+}$

(b) $\text{FeS}_{(\text{s})} + \text{NO}_3^{-} \rightarrow \text{NO}_{(\text{g})} + \text{Fe}_{(\text{aq})}^{3+} + \text{SO}_4^{2-} \text{ (aq)}$

(c) $\text{Sn}_{(\text{s})} + \text{NO}_3^{-} \text{ (aq)} + \text{Cl}_{(\text{aq})}^{-} \rightarrow \text{SnCl}_6^{2-} \text{ (aq)} + \text{NO}_2 \text{ (g)}$

Answers **5.1** C₆H₆ is the solute **5.3** NH_{3(l)} (polar) **5.5** (a) C₆H_{14(l)} (nonpolar) (b) CH₃CH₂CH₂OH_(l) (polar) (c) C₅H_{10(l)} (nonpolar) (d) C₆H₅CH_{3(l)} (nonpolar) (e) CH₃CH₂OH_(l) (polar) (f) C₆H₅NH_{2(l)} (polar) **5.7** Soap are salts of oils and therefore are overall non-polar molecules. Soaps are produced by mixing an oil with a strong base. **5.9** 23% **5.11** 0.1 g **5.13** 20mL **5.15** 0.062g **5.17** 100 mL **5.19** 25mL **5.21** AgNO₃(Soluble); AgBr (Insoluble); CaCO₃(Soluble);Na₂CO₃(Soluble) **5.23** (a) Ca(OH)₂ (Ca²⁺ + 2 OH⁻) (b) K₂CrO₄ (2 K⁺ + CrO₄²⁻) (c) Ca(NO₃)₂ (Ca⁺ + 2 NO₃⁻) **5.25** (a) Acid-base (b) Precipitation (c) redox **5.27** 2 H⁺_(aq) + 2 OH⁻_(aq) → 2 H₂O_(l) **5.29** (a) Fe_(s) + O_{2(g)} → Fe³⁺_(aq) + O²⁻_(aq) (b) Precipitation **5.31** 2 MnO₄⁻_(aq) + 2 H⁺ + 3 SO₃⁻²_(aq) → H₂O_(l) + 2 MnO_{2(s)} + 3 SO₄⁻²_(aq) **5.33** No solution listed

6

Reactions in gase phase



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THE air we all breath 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.

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GOALS

- 1 Use the ideal and real gas law
- 2 Calculate partial pressures
- 3 Compute gas-property changes
- 4 Carry stoichiometric calculations with volumes
- 5 Compute root square mean velocities

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 by means of weak forces. Solids on the other hand are packed materials and its 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 of the combination of two atoms of the same element. For example, molecular oxygen (O_2) is 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 of 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 gas state.

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Discussion: Explain why a hot air balloon rises up. Furthermore, why a He-filled birthday balloon rises while if you fill it with air it does no?

Characteristics of gases Gases has different properties compared to solids of liquids:

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- Gases assume the volume and shape of its container. As they expand, they have no shape different than their container's shape.
- Gases are compressible: they can be compressed, reducing its volume. Differently, liquids and solids are incompressible.
- The density of gases is small, compared to the one for solids and liquids.

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Volume, V The volume of a gas (V) is the amount of space it occupies, and gases fully occupy the volume of its container. Liters (L) and milliliters (mL) are units of volume. Liter is a cubic unit and one litter equals to 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

$$T_K = T_C + 273$$

1290 *Amount of gas, n* The amount of a gas (n) refers to the quantity of gas particles. The larger the amount of gas, the larger the amount of gas particles. The amount of gas is measured in moles or grams. Figure 6.1 displays a list of all gas elements.

Figure 6.1: 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 its movement, they frequently hit the walls of its container, like the raindrops hitting the ceiling when it rains. When they hit the walls they exert a pressure, and pressure is defined as the force acting on certain area. The larger pressure the stronger the collisions with the walls and the higher the frequency of collision—the stronger the force applied on the walls. Imagine you are driving a motorcycle. While you drive you can feel the collision of the air's particle with your face. The faster you go the higher pressure. The value of air's 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 the 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 with respect to the sea level, the lower the air pressure. The weather also affects pressure, and in hot days the pressure of air is higher, whereas on a cold day pressure is lower.

Units of pressure are: bars, atmospheres (atm), torr, pascals (Pa) or millimeters of mercury (mmHg). In order to convert pressure units, you can use the following conversion factors:

$$\frac{1 \text{ atm}}{1.01325 \text{ bar}}$$

$$\frac{1 \text{ atm}}{760 \text{ mmHg}}$$

$$\frac{1 \text{ torr}}{1 \text{ mmHg}}$$

$\frac{1 \text{ atm}}{101325 \text{ Pa}}$

one millimeters 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.



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Figure 6.2: Examples of gases

Sample Problem 53

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

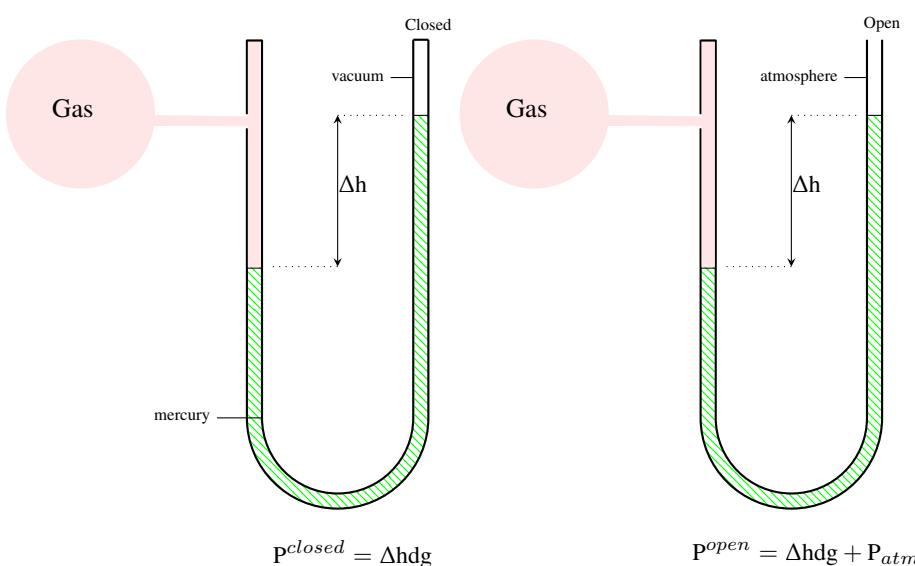
An oxygen sample has a pressure of 730 mmHg. Convert this value to atmospheres.

Answer: 0.96 atm.

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1300

Figure 6.3: Two types of manometers: open-tube and closed-tube manometer



The pressure exerted by a gas changes level of mercury on both sides of the tube and the difference in height 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 pressures below the atmospheric pressure—when the gas pressure increases the left

1305

column of the barometer is reduced and the right column increases. The difference between both columns is related to the gas pressure by means of:

$$P_{closed} = h \cdot g \quad P_{open} = h \cdot g + P_{atm} \quad (6.1)$$

1310 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

1315 P_{atm} is the atmospheric pressure close to 101325 Pa

1320 For the open-tube manometer, normally used to measure pressures above the atmospheric pressure, we need to take into account the atmospheric pressure to the gas pressure. For this type of manometers, if the left column is below the right column ($\Delta h = h_{right} - h_{left} < 0$), this means that the pressure of the gas is below the atmospheric pressure.

▼ A barometer used to measure the atmospheric pressure



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▼ A manometer used to measure gas pressures



© wikipedia

▼ A pressure gauge



© PxFuel

Figure 6.4: Pressure measuring devices

6.2 Ideal gas law

1325 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 by the ideal gas law. In this section we will introduce this law in two different forms: in terms of volume and in 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

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 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.

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Sample Problem 54

Helium gas is used to inflate blimps, scientific balloons and party balloons. What is the volume in liters of a 0.2 moles of Helium balloon at 300K and 2 atm.

SOLUTION

Analyze the Problem	Given	Asking
	$T = 300\text{K}$ $P = 2\text{atm}$ $n = 0.2\text{mol}$ $R = 0.082 \frac{\text{atm} \cdot \text{L}}{\text{mol} \cdot \text{K}}$	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.

Answer: 77.00 atm.

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:

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 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

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 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 55

What is the density of 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.

Answer: 19.87 g/mol.

STP conditions STP conditions refer to standard temperature (273K) and pressure (1 atm) conditions. Working at STP conditions means pressure will be fixed at 1 atm and temperature at 273K.

(1 atm and 273K) **STP Conditions**

Sample Problem 56

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.

Answer: 5g.

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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.

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Solving problems with an initial and final state In order 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 the situation in which you have a 1L hot air balloon with 1 moles of a 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 moles of gas and the final estate corresponds to an unknown volume and 5 moles. Using the ideal gas formula twice you have:

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$$\left. \begin{array}{l} PV_1 = n_1 RT \\ PV_2 = n_2 RT \end{array} \right\} \frac{PV_1}{PV_2} = \frac{n_1 RT}{n_2 RT} \quad (6.2)$$

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as some of the variables of the cancel out:

$$\frac{P'V_1}{P'V_2} = \frac{n_1 RT}{n_2 RT} \quad (6.3)$$

and you end up with Avogadros' law. If you plug the numbers into the formula:

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$$\frac{1L}{V_2} = \frac{1 \text{ mol}}{5 \text{ mol}} \quad (6.4)$$

and you get a final volume of 5L.

Sample Problem 57

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:

Analyze the Problem	Given	Asking
	$V_1 = 3L$ $P_1 = 5 \text{ atm}$ $P_2 = 10 \text{ atm}$	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

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.

Answer: 2.66 atm.

Pressure-Volume change If temperature and the number of moles of a 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:

$$\boxed{\frac{P}{V} = c \quad \text{or} \quad P_1 \cdot V_1 = P_2 \cdot V_2} \quad \text{Boyle's law}$$

where:

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P_1, V_1 are the initial pressure and volume

P_2, V_2 are the final pressure and volume

c is a constant

Volume-Temperature change Imagine you cool down a balloon at fixed pressure (under the atmosphere). What would happen to the balloon's volume? Based on Charle's law, its volume will decrease:

$$\boxed{\frac{V}{T} = c \quad \text{or} \quad \frac{V_1}{T_1} = \frac{V_2}{T_2}} \quad \text{Charle's law}$$

where:

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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 balloon. 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

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Relating the different variables of a gas The question is now, if we increase the pressure at 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 increase at fixed pressure and volume, will the temperature of the gas increase or perhaps decrease. We can answer these questions by means of the ideal gas law. If the variables that we need to relate are in the same side of the equation (e.g. P and V) then if one of the variables increase the other will decrease. Differently, If the gas variables to relate are located in 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 in 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 in opposite sides of the ideal gas law ($PV = nRT$), if P increases, T will increase as well.

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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.

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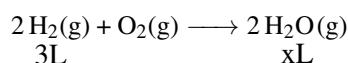
Molar volume If we work at STP conditions the volume of one mole of gas equals to 22.4L, and we refer to this relationship as the molar volume.

$$\frac{1\text{mol}}{22.4 \text{ L at STP}}$$

Molar Volume

This relationship allows us to carry stoichiometric calculations in chemical reaction involving gases.

stoichiometry and gases If you encounter chemical reactions with gases, the molar volume relation allows you to carry stoichiometric calculations. Why is this important? Imagine you have this reaction:



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Gases are measured by means of their pressure and is 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. In order 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 is mol. If the reaction deals with gases you want to interpret the stoichiometric coefficients in terms of liters. This way:

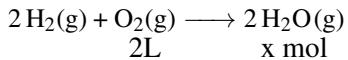
$$x = 3 \cancel{\text{L of H}_2} \times \frac{2 \text{ L of H}_2\text{O}}{2 \cancel{\text{L of H}_2}} = 3 \text{ L of H}_2\text{O}.$$

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.

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Sample Problem 58

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

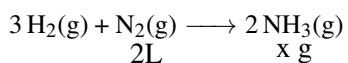
We will solve the problem in a single line, first relating the liters of oxygen and liters of water produced and finally converting liters of water into moles of water using the molar volume. Remember when there are gases in the reaction, the stoichiometric coefficients can be interpreted in terms of 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 at STP conditions according to the following equation:



Calculate the number of grams of ammonia produced from 0.5L of nitrogen.

Answer: 5g.

Partial and total pressure Imagine you have a container with 1atm of Ar, and another container of the same volume containing 1 atm of Ne. If you combine the containers into a single container (and 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:

$$P_{\text{Total}} = p_1 + p_2 + \dots + p_n \quad \text{Dalton's Law}$$

Sample Problem 59

Medical Air is a 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.

Answer: 4 atm.

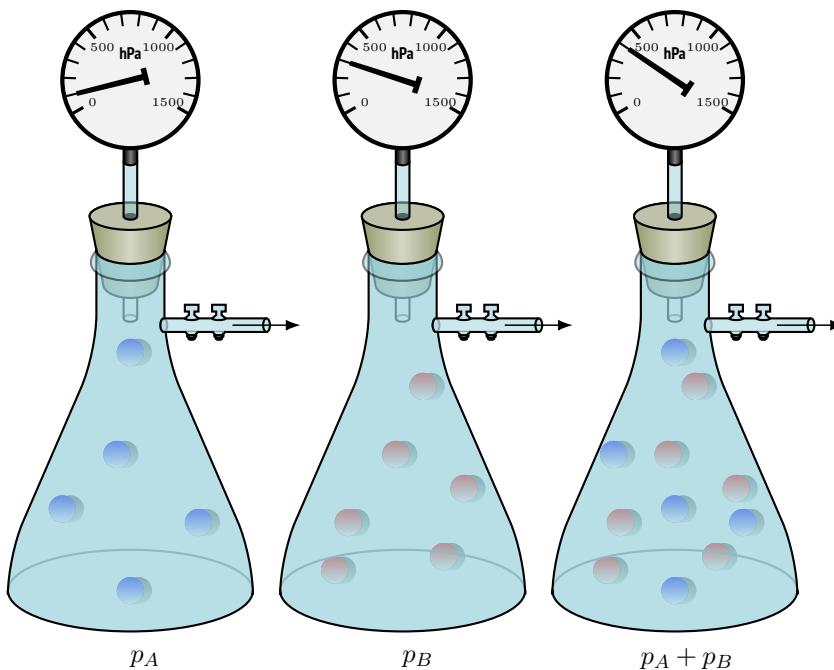


Figure 6.5: A visual representation of Dalton's law of partial pressure: after adding two different gases with different partial pressures, the final pressure is the result of adding both partial pressures.

In Figure 6.5, we have that after combining two gases with different partial pressures the resulting pressure is the addition of both partial pressures.

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

$$p_A = \frac{n_A R T}{V}$$

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 with respect to all components. 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 60

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

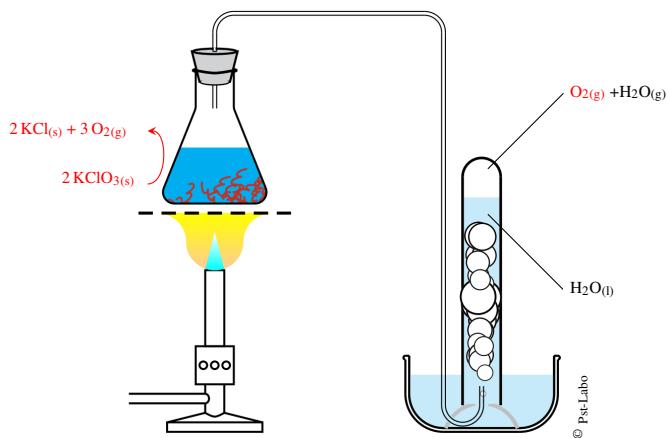
A mixture of gases with a total pressure of 5 atm contains 1 mol of Ar and 1 mol of He. Calculate the partial pressure of each component on the mixture.

Answer: $p_{Ar}=2.5\text{ atm}$, $p_{He}=2.5\text{ atm}$.

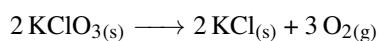
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Figure 6.6: Apparatus for measuring the amount of gas produced by a reaction over water.

Collecting gas over water: use of partial pressures



Numerous reactions produce gases. As an example, potassium chlorate decomposes to produce oxygen gas:



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The volume of gas produced by a chemical reaction is collected often times over water. Gas bubbles go through water being collected in an apparatus similar to the one represented in Figure 6.6.

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 another 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:

$$P_{\text{gas}} = P_{\text{total}} - P_{\text{H}_2\text{O}}$$

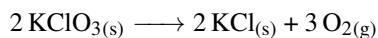
The partial pressure of water, also called the vapor pressure of water, depends on temperature and its values can be found in Table 6.1. For example, at 25°C, the vapor pressure of water in the atmosphere is 0.0313 atm and at 100°C is equal to 1 atm. When liquids boil, their vapor pressure is equal to the atmospheric pressure, that is the reason behind the vapor pressure of water being 1 atm at 100°C, the boiling point of water. 1430

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

Sample Problem 61

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.

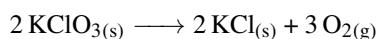
SOLUTION

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 KClO₃ decomposed.

Answer: 1.2×10^{-4} moles of KClO_3 .

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6.5 Real gases and the kinetic molecular theory of gases

Until now we have discussed ideal gases. Ideal gases represent very diluted gases in which the gas particles do not see each other, as they are apart. The particles of an ideal gas are very minute without a volume. The collisions between the particles and the walls of the container are elastic—this means the gas 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. We will also discuss the kinetic molecular theory with a particular emphasis on particle average velocity—this is technically called root mean square velocity, v_{RMS} .

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 do 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 $\text{L}\cdot\text{mol}$

The meaning of the Van der Waals constants There are two Van der Waals constants: a and b . 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 H_2O 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 are very weak and in contrast, the interactions between the particles of H_2O 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.

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Table 6.2 Van der Waals constants for several gases

gas	a (atm · L ² / mol ²)	b (L/mol)	gas	a (atm · L ² / mol ²)	b (L/mol)
NH ₃	4.225	0.0371	Ar	1.355	0.03201
C ₆ H ₆	18.24	0.1154	CO	3.640	0.04267
CH ₄	2.283	0.0427	CH ₃ OH	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

Sample Problem 62

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 $b = 0.0371 \text{ L/mol}$.

Answer: 664 atm; 659 atm.

Kinetic theory of gases The kinetic theory of gases is a model that explain 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 collide with the walls of its container exerting pressure.
- Gas particles are far apart from each other, barely interacting.
- The average kinetic energy of the particles of a gas (this is the energy of the particles due to movement) is proportional to the temperature of the gas.

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By means of 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 its 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 explain

1475

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 an experimental law; 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:

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$$v_{RMS} = \sqrt{\frac{3000RT}{MW}}$$

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 $8.314 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

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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 63

Order the following molecules in increasing order of root mean square velocity:

Ne, CO_2 and H_2O .

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($MW=20\text{g/mol}$), CO_2 ($MW=44\text{g/mol}$) and H_2O ($MW=18\text{g/mol}$). 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 .

Answer: 625m/s .

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Distribution of velocities The root mean 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 a gas follow a distribution which is mass and temperature dependent. As shown in Figure 6.7, 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.

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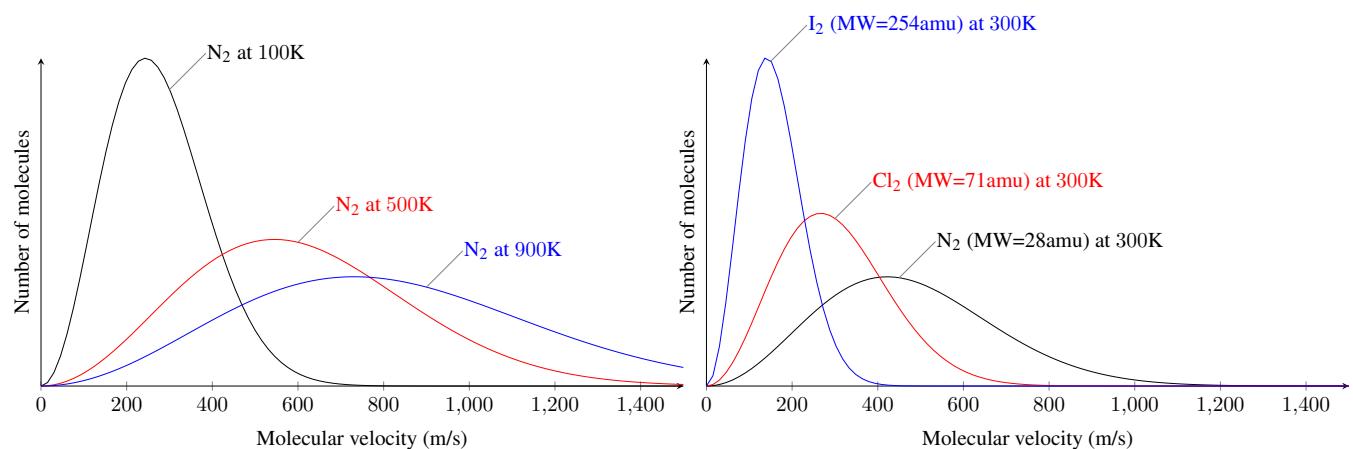


Figure 6.7: Effect of temperature and mass on the distribution of molecular speeds

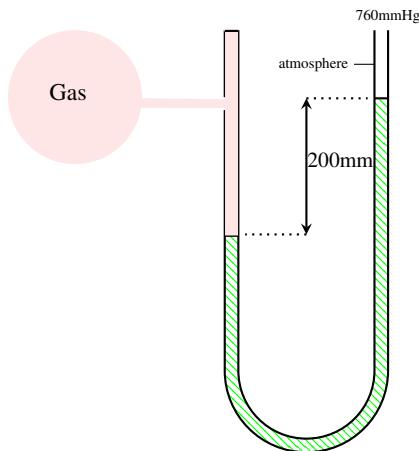
CHAPTER 6

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

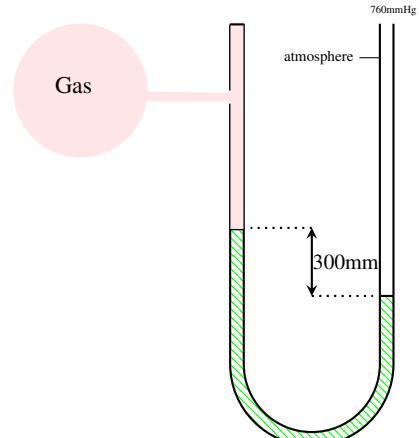
6.2 Convert the following properties: (a) A pressure value of 900 mmHg into torr (b) A temperature value of 400K into °C

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) Given that the height of the column is 750mm, calculate the atmospheric pressure in MPa. (b) 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. (c) What are the benefits of building a barometer with a lighter liquid than mercury? (d) What are the drawbacks of building a barometer with a lighter liquid than mercury?

IDEAL GAS LAW

6.6 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.

6.7 Dinitrogen oxide, used in dentistry, is an anesthetic also called laughing gas. What is the pressure in atm of 0.35 moles of N₂O at 22°C in a 5L container?

6.8 A 4 moles sample of gas at 400K has a pressure of 10 atm. Calculate the volume of the sample.

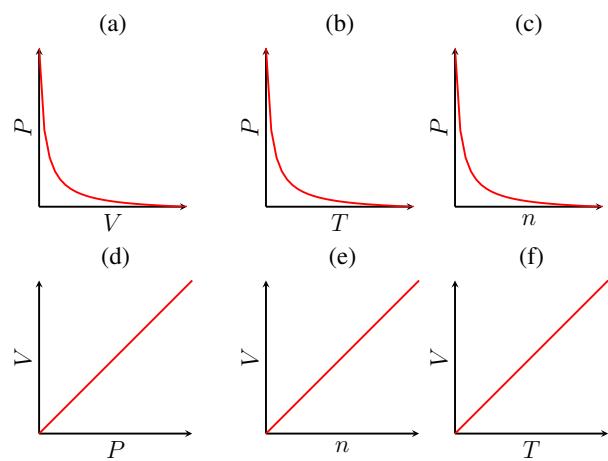
6.9 A 3 grams sample of Ar at 40°C is placed in a 3L container. Calculate the pressure inside the container.

6.10 Eighteen moles of a gas in a 11L container at 400K exert a pressure of 3 atm. Calculate the molar mass of the gas.

6.11 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.

6.12 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)

6.13 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

6.14 A sample of a gas at 400K and 12 atm is cooled in the same container to 200K. Calculate the new pressure.

6.15 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.

6.16 A 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.

6.17 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.

6.18 If the pressure of a gas increases, at fixed temperature and moles, its volume....

6.19 If the temperature of a gas increases, at fixed volume and moles, its pressure....

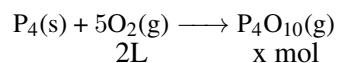
MIXTURE OF GASES AND GAS STOICHIOMETRY

6.20 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?

6.21 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?

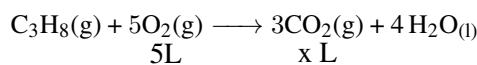
6.22 The atmospheric pressure on a hot day is 780 mmHg. Given that the air is made of 78% of nitrogen and 22% of oxygen, calculate the partial pressure of each gas in the air.

6.23 Phosphorus reacts with oxygen gas to produce tetrephosphorus decaoxide according to the following equation:

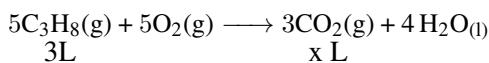


Calculate the number of moles of phosphorus that react with 2L of oxygen at STP conditions.

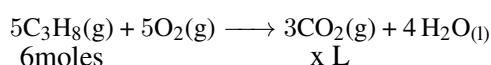
6.24 For the following reaction, calculate the unknown *x* at STP conditions:



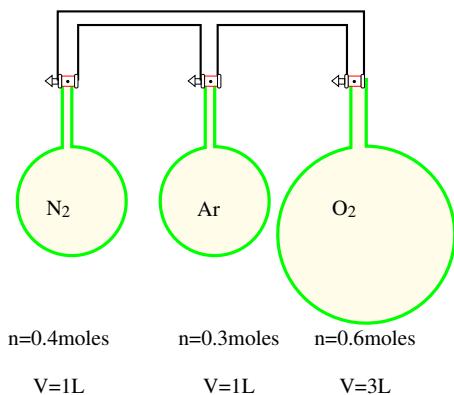
6.25 For the following reaction, calculate the unknown *x* at STP conditions:



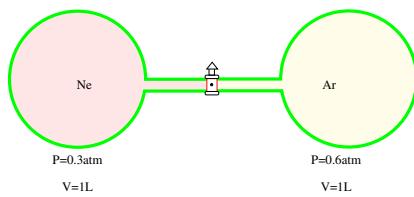
6.26 For the following reaction, calculate the unknown x at STP conditions:



6.27 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



6.28 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.



REAL GASES AND THE KINETIC MOLECULAR THEORY OF GASES

6.29 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 $b = 0.0237\text{L/mol}$

6.30 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 $|p^{ideal} - p^{real}| / p^{real} \times 100$.

6.31 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

6.32 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

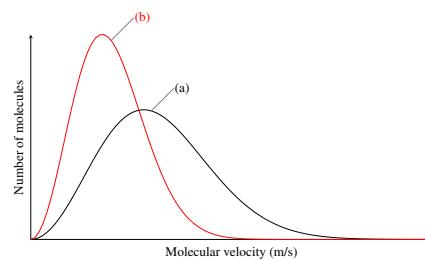
6.33 What is the rms speed of O_2 at STP?

6.34 Order the following molecules in increasing order of root-mean square velocity: Ne , CO_2 , H_2O , CH_4 .

6.35 The kinetic molecular theory of gases assumes that:

- (a) gas particles interact with each other
- (b) gas particles have large sizes
- (c) particles move slowly
- (d) gas particles move randomly

6.36 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?



Answers **6.1** (a) 1520 mmHg (b) 2.96×10^{-2} atm (c) 298K **6.3** (a) higher (b) 0.127MPa (c) 960mmHg
6.5 (a) 0.09MPa (b) 8.7×10^{-3} atm (c) it would be more sensitive to pressure changes (d) it would have to be taller than a barometer based on mercury **6.7** 1.7atm **6.9** 0.64 atm **6.11** 21 g/mol **6.13** (a) (b) (f) (c) (e) **6.15** 30L **6.17** 2.8 L **6.19** increases **6.21** 1.5atm **6.23** 0.017 mol **6.25** 1.8L **6.27** (a) $p_{N_2}=1.97\text{atm}$, $p_{Ar}=1.48\text{atm}$, $p_{O_2}=2.95\text{atm}$ (b) 6.40 atm **6.29** (a) 49.2 atm (b) 50.36 atm **6.31** (a) Ar (b) CO **6.33** 481.9 m/s **6.35** gas particles move randomly



7

Thermochemistry

ENERGY involves many aspects of our everyday life. Chemical reactions happening in our body consume or release energy as we walk, study, and even breath. We also use energy at home to warm food or turn on the lights, to 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 of energy. Similarly, the burning of fossil fuels such as oil, propane, or gasoline provides enough energy to maintain our homes. Some reactions produce energy whereas others release energy. On the other hand, how do we measure the energy released or consumed in a reaction? Thermochemistry is the study of heat in chemical reactions. This chapter will answer this and other questions as it covers different aspects of thermochemistry that involves the interaction between chemistry and energy. You will learn about temperature, heat and how to quantitatively compute the energy exchanged during a chemical reaction.

7.1 Energy & temperature

When you are running, walking, dancing, or thinking, you are using energy to do work. In fact, 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



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GOALS

- 1 Convert heat to temperature rise
- 2 Carry calorimetric calculations
- 3 Use the enthalpy table
- 4 Compute enthalpy changes
- 5 Apply Hess's Law to compute enthalpy

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Discussion: What do you think about renewable energy? List three benefits and three inconveniences of renewable sources of energy.

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substance receives heat it gets warmer and it raises its temperature, whereas if it loses heat it gets cooler and its temperature decreases.

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▼Flowers convert sunlight into chemical energy



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▼a bullet has kinetic energy



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▼water on a dam has potential energy



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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 to joules and joules to calories using the following conversion factor:

$$1\text{cal} = 4.184\text{J} \quad \text{or} \quad \frac{1\text{cal}}{4.184\text{J}} \quad (7.1)$$

▼thermal energy refers to heat



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Figure 7.1: Examples of different types of energy

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. In order 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 is 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 being 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 to joules and joules to calories using the following conversion factor:

Sample Problem 64

Convert the following energy values:

- (a) 50000 cal to Kcal (b) 48000 J to cal

SOLUTION

We will use the conversion factor for kilo and the relationship between calorie and joule:

$$(a) 50000\text{cal} \times \frac{1\text{kcal}}{1000\text{cal}} = 50\text{kcal}; (b) 48000\text{J} \times \frac{1\text{cal}}{4.184\text{J}} = 11472.2\text{cal}.$$

◆ STUDY CHECK

Convert the following energy units:

- (a) 200 cal to Kcal (b) 7000 J to cal

Answer: (a) 0.2Kcal; (b) 1673 cal.

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

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1575 use the formulas below:

$$T_F = 1.8T_C + 32$$

$$T_F = 1.8T_K - 459.4$$

$$T_K = T_C + 273$$

(7.2)

Sample Problem 65

Convert 25 °C to °F.

SOLUTION

- 1 Step one: list of the given variables.

Analyze the Problem	Given	Asking
	$T_c = 25^\circ C$	T_F

- 2 Step two: use the formula $T_F = 1.8T_C + 32$ to convert from °C to °F.

$$T_F = 1.8T_c + 32$$

- 25° 3 Step three: solve for $T_F = 1.8 \times 25 + 32 = 77^\circ F$.

◆ STUDY CHECK

Convert 200°C to K.

Answer: 473K.

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.

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7.2 The first law of thermodynamics. From energy to temperature

Materials can absorb heat and receive work. On one hand, think about a pizza in your oven, or a cup of milk in the microwaves. These substances receive heat from the oven or in form of microwaves and they become hot. Heat transforms in an increase of 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 . Heat transform in a temperature change. Some substances like metals are able to increase its temperature very quickly with a small amount of heat received, whereas others need a larger amount of heat to rise up its temperature. Think about why you use oil to deep fried food? Why not using water? First of all, oil can rise its temperature very quickly and on top of that it does not boil easily.

Work Think about what happens at a car's engine. In an engine, chemical energy is converted in movement and with this movement, a car is able to 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

$$W = -P \cdot \Delta V \quad (7.3)$$

where:

W represent 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 words, 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 change in volume at constant pressure is normally called PV work.

Sample Problem 66

Calculate the work (in $L \cdot atm$) involved in the expansion of a gas from 10L to 20L at constant external pressure of 2atm. Convert the value in joules using $1J=101.3L \cdot atm$.

SOLUTION

We will use Equation 7.3 that related work with pressure and volume change:

$$W = -P \cdot \Delta V = -2atm \cdot (20 - 10)L = -20L \cdot atm$$

If we convert this value into J:

$$-20L \cdot atm \times \frac{1J}{101.3L \cdot atm} = -0.2J$$

As the value is negative, it means that the system gives away work.

❖ STUDY CHECK

Calculate the work (in $\text{L} \cdot \text{atm}$) involved in the compression of a gas from 10L to 5L at constant external pressure of 5atm. Convert the value in joules using $1\text{J}=101.3\text{L} \cdot \text{atm}$.

Answer: $25\text{L} \cdot \text{atm}, 0.24\text{J}$.

Heat capacity The heat capacity c of a material is defined as:

$$c = \frac{\text{heat adsorbed}}{\text{temperature increase}} \quad (7.4)$$

The heat capacity is a characteristic property of each material that indicates the energy required to rise its temperature and can be expressed in $\text{cal}/^\circ\text{C}$ or $\text{J}/^\circ\text{C}$ units. As this property depends on the amount of matter, often times the heat capacity is expressed per mass as the specific heat capacity (c_e) or mole unit as the molar heat capacity c_m . For example, the specific heat of water is $1\text{cal/g}^\circ\text{C}$ that is the same as $4.184\text{J/g}^\circ\text{C}$. That means that we need to give 1 calorie in order to warm up one gram of water 1°C . Similarly, the specific heat of aluminum, a metal, is $0.2\text{cal/g}^\circ\text{C}$ or $0.89\text{J/g}^\circ\text{C}$; that means the energy needed to rise 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 in order to increase the temperature of a gram of water in 1°C , whereas we need to give 0.2 cal in order to increase the temperature of a gram of aluminum in 1°C . Why are these two numbers so different? The answer is because 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. Mind the specific heat if water is a well known value that you need to be familiar with:

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$$c_e^{\text{H}_2\text{O}} = 4.184\text{J/g}^\circ\text{C} \quad \text{or} \quad c_e^{\text{H}_2\text{O}} = 1\text{cal/g}^\circ\text{C} \quad (7.5)$$

Table 7.1 Values of specific heat for different materials

Material	Specific heat ($\text{J/g}^\circ\text{C}$)	Material	Specific heat ($\text{J/g}^\circ\text{C}$)
$\text{H}_2\text{O(l)}$	4.184	Fe(s)	0.444
ethyl alcohol _(l)	2.460	Au(s)	0.129
vegetable oil _(l)	1.790	Cu(s)	0.385
$\text{NH}_3\text{(l)}$	4.700	$\text{H}_2\text{O(s)}$	2.010
Dry Air _(g)	1.0035	$\text{CO}_2\text{(g)}$	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 microwaves, 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:

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$$Q = m \cdot c_e \cdot (T_f - T_i) \quad (7.6)$$

where:

Q is the amount of heat received, either in cal or J.

m is the mass of material in grams

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c_e is the specific heat of the material (in $\text{cal/g}^\circ\text{C}$ or $\text{J/g}^\circ\text{C}$)

$T_f - T_i = \Delta T$, 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 67

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

- 1 **Step one:** list of the given variables.

Analyze the Problem	Given	Asking
	$c_e = 0.214 \frac{\text{cal}}{\text{g}^\circ\text{C}}$ $m = 45.2\text{g}$ $T_{\text{initial}} = 25^\circ\text{C}$ $T_{\text{final}} = 50^\circ\text{C}$	Q

- 2 **Step two:** use the formula $Q = m \cdot c_e \cdot (T_{\text{final}} - T_{\text{initial}})$ to temperature increase to heat absorbed:

$$Q = m \cdot c_e \cdot (T_{\text{final}} - T_{\text{initial}})$$

- 3 **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 .

Answer: $Q = 231\text{cal}$.

First law of thermodynamics: the internal energy The combination of work (W) and heat (Q) is called internal energy (ΔE):

$$\Delta E = Q + W$$

(7.7)

The first law of thermodynamics—the law of conservation of energy—states that the energy of the universe is constant.

Sample Problem 68

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 7.3 that related work with pressure and volume change. As the resulting unit of work will be $\text{L} \cdot \text{atm}$, 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 atmosphere 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.

Answer: $-9.5 \times 10^6\text{J}$.

7.3 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. This section will show you how to carry calorimetric calculations.

The calorimeter A calorimeter is 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. In the contrary, if the temperature inside a calorimeter decreases, this means that the reaction consumes energy. There are two different types of calorimeters: constant-pressure and constant-volume calorimeters. As a note, ΔQ_r is called molar heat of reaction as it represents energy per mole, with units of kJ/mol .

Exothermic and endothermic reactions Some reactions release heat and are called exothermic. Others absorb heat and are called endothermic. Think for example the combustion of the gas in a cooking stove, it produces heat and hence the

chemical reaction happening is exothermic. Differently, if you cook bread, it needs heat to rise. Similarly, if you melt an ice cube you need to give energy to the cube so that it becomes water. These are examples of endothermic reactions. Endothermic reactions have positive ΔQ_r whereas exothermic reactions have negative ΔQ_r .

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 introduce 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:

$$0 = n \cdot \Delta Q_r + \Delta Q_{\text{water}} \quad \text{constant pressure}$$

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 to 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 69

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
	$n = 5 \times 10^{-3} L$ $0.5M = 2.5 \times 10^{-3}$ moles $V = 10mL$ $d = 1g/mL$ $T_f = 27^\circ C$ $T_i = 25^\circ C$ $c_e^{\text{H}_2\text{O}} =$ $4.184\text{J/g}^\circ\text{C}$	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:

$$0 = n \cdot \Delta Q_r + V \cdot d \cdot c_e^{\text{sol}} \cdot (T_f - T_i)$$

$$0 = 2.5 \times 10^{-3} \text{ mol} \cdot \Delta Q_r + 10g \cdot 4.184\text{J/g}^\circ\text{C} \cdot (27^\circ\text{C} - 25^\circ\text{C})$$

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 $4.184\text{J/g}^\circ\text{C}$.

Answer: 27.39°C .

1695 *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 calorimeters are rigid and even if gas is produced the volume of the container will not change—that is why 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.

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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:

$$0 = n \cdot \Delta Q_r + \Delta Q_{\text{water}} + \Delta Q_{\text{walls}}$$

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:

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ΔQ_r is the heat exchanged due to a chemical reaction in J/mol

n is the number of moles 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: $4.184\text{J/g}^\circ\text{C}$

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c^{cal} is the heat capacity of the calorimeter also known as calorimeter factor

$T_f - T_i = \Delta T$, is the temperature change from the initial to the final temperature

Sample Problem 70

A 3 mol-sample of a chemical is burned in a constant-volume calorimeter with 10g of water and a heat capacity of $10\text{KJ}/^\circ\text{C}$. 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

	Given	Asking
Analyze the Problem	$n = 3\text{mol}$ $m = 10\text{g}$ $T_f = 40^\circ\text{C}$ $T_i = 25^\circ\text{C}$ $c^{\text{cal}} = 10^4\text{J}/^\circ\text{C}$ $c_e^{\text{H}_2\text{O}} = 4.184\text{J/g}^\circ\text{C}$	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 $\text{KJ}/^\circ\text{C}$, whereas the units of the specific heat of water are $\text{J/g}^\circ\text{C}$ and hence, we need to convert KJ into J ; that is the reason we use $10000\text{J}/^\circ\text{C}$ 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 $11\text{KJ}/^\circ\text{C}$. Calculate the heat of reaction knowing that the temperature of water inside the calorimeter rises 10°C .

Answer: -55KJ/mol .

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▼A constant-volume calorimeter



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▼A constant-pressure calorimeter



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Figure 7.2: 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.

7.4 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.

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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 at 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.

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Table of standard enthalpies The values of enthalpies are tabulated at the end of the chapter. 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 this table. If you look for the standard enthalpy of C—an element—from the table you might find several values. The values of graphite carbon is $\Delta H_f^\circ = 0\text{KJ/mol}$. Differently, the values for diamond carbon is 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.

1730 Let us find the standard enthalpy for molecular nitrogen, $\text{N}_2(\text{g})$ —another element. If you look into the table 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 the table, the value is also $\Delta H_f^\circ = 0\text{KJ/mol}$.

1735 The rule of thumb is: elements on its natural state have zero H_f° . Below we will explain more about the meaning of natural state. Now, look for the standard enthalpy of carbon monoxide gas, $\text{CO}(\text{g})$. The value should not be zero, as carbon dioxide is not an element and is made of two different types of atoms. Indeed, in the table we find $\Delta H_f^\circ(\text{CO}(\text{g})) = -110.5\text{KJ/mol}$.

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Sample Problem 71

Using the enthalpy tables at the end of the chapter, locate the enthalpy values for: $\text{CaS}_{(\text{s})}$, $\text{AlCl}_3_{(\text{s})}$ and $\text{H}_2\text{O}_{(\text{l})}$.

SOLUTION

The enthalpy of calcium sulfide in solid state ($\text{CaS}_{(\text{s})}$) is -482.4KJ/mol . For the case of aluminum chloride in solid state too ($\text{AlCl}_3_{(\text{s})}$), 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: $\text{I}_{2(\text{aq})}$, $\text{F}_{2(\text{g})}$ and $\text{C}_{\text{diamond}(\text{s})}$.

Answer: 23, 0, 1.9KJ/mol .

1745 *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 $\Delta H_f^\circ(\text{Al}_{(\text{g})}) = 314\text{KJ/mol}$, whereas $\Delta H_f^\circ(\text{Al}_{(\text{s})}) = 0\text{KJ/mol}$. In general, for metals, its natural state is solid. For non-metallic elements, such as hydrogen, oxygen, nitrogen, fluorine, chlorine, its natural state is in the form of a diatomic gas molecule. For example, $\Delta H_f^\circ(\text{H}_{2(\text{g})}) = 0\text{KJ/mol}$, $\Delta H_f^\circ(\text{N}_{2(\text{g})}) = 0\text{KJ/mol}$ or $\Delta H_f^\circ(\text{O}_{2(\text{g})}) = 0\text{KJ/mol}$. For the case of carbon, its natural state is graphite, $\Delta H_f^\circ(\text{C}_{\text{graphite}(\text{s})}) = 0\text{KJ/mol}$. 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.

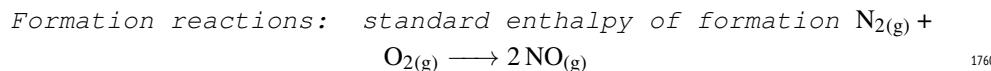
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Table 7.2 Standard states for different elements. For all $\Delta H_f^\circ = 0\text{KJ/mol}$

Element	Standard state	Element	Standard state
Hydrogen	$\text{H}_2(\text{g})$	Oxygen	$\text{O}_2(\text{g})$
Nitrogen	$\text{N}_2(\text{g})$	Chlorine	$\text{Cl}_2(\text{g})$
Iron	$\text{Fe}(\text{s})$	Aluminium	$\text{Al}(\text{s})$
Carbon	$\text{C}_{\text{graphite}}(\text{s})$	Phosphorus	$\text{P}_4(\text{s})$
Fluorine	$\text{F}_2(\text{g})$	Bromine	$\text{Br}(\text{l})$
Mercury	$\text{Hg}(\text{l})$	Sulfur	$\text{S}_8(\text{s})$
Iodine	$\text{I}_2(\text{s})$	Silicon	$\text{Si}(\text{s})$

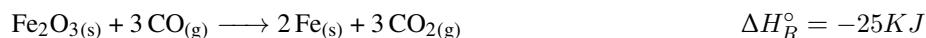
The formation reaction starts with natural-state elements (e.g. H_2 , N_2 , etc.) to form a chemical. For example, the formation reaction of NO is given by:



On the products side we have the chemical formed (NO) whereas on the reactant side we have the elements that make NO on its natural state (H_2 and N_2). The enthalpy associated with this reaction is called standard enthalpy of formation $\Delta H_f^\circ(\text{NO}(\text{g}))$. 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 on its natural state: $\text{CO}(\text{g})$ and $\text{Fe}_2\text{O}_3(\text{s})$ has enthalpies different than zero. For this reason, the second enthalpy is labeled as ΔH_R° , and is called standard enthalpy of reaction.

Standard enthalpy change for a reaction In order 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:

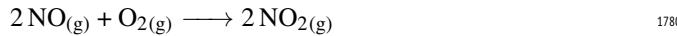
ΔH_R° is the standard enthalpy change of the reaction

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$\Delta H_{\text{products}}^\circ$ 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:

$$\begin{aligned}\Delta H_R^\circ &= \Delta H_{products}^\circ - \Delta H_{reactants}^\circ = \\ &= [2 \cdot \Delta H_f^\circ(\text{NO}_{2(g)})] - [2 \cdot \Delta H_f^\circ(\text{NO}_{(g)}) + \Delta H_f^\circ(\text{O}_{2(g)})] = \\ &= [2 \cdot 33.2] - [2 \cdot 90.29 + 0] = -114\text{KJ}\end{aligned}$$

This reaction is exothermic and releases heat.

Sample Problem 72

Using the enthalpy table, calculate ΔH_R° for the following reactions:

- (a) $4 \text{H}_{2(g)} + \text{O}_{2(g)} \longrightarrow 2 \text{H}_{2\text{O(l)}}$
- (b) $3 \text{H}_{2(g)} + \text{N}_{2(g)} \longrightarrow 2 \text{NH}_{3(g)}$
- (c) $2 \text{Al}_{(s)} + 3 \text{Cl}_{2(g)} \longrightarrow 2 \text{AlCl}_{3(s)}$

SOLUTION

In order to answer all questions, we need a set of ΔH_f° values: $\Delta H_f^\circ(\text{H}_{2(g)})$, $\Delta H_f^\circ(\text{O}_{2(g)})$, $\Delta H_f^\circ(\text{N}_{2(g)})$, $\Delta H_f^\circ(\text{Al}_{(s)})$ are all zero, whereas $\Delta H_f^\circ(\text{H}_{2\text{O(l)}}) = -285.8\text{KJ/mol}$, $\Delta H_f^\circ(\text{NH}_{3(g)}) = -45.0\text{KJ/mol}$ and $\Delta H_f^\circ(\text{AlCl}_{3(s)}) = -705.63\text{KJ/mol}$. For the first example, we have:

$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{H}_{2\text{O(l)}})] - [4 \cdot \Delta H_f^\circ(\text{H}_{2(l)}) + \Delta H_f^\circ(\text{O}_{2(g)})] \\ &= [2 \cdot -285.8] - [4 \cdot 0 + 0] = -572\text{KJ}\end{aligned}$$

For the second example:

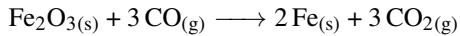
$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{NH}_{3(g)})] - [2 \cdot \Delta H_f^\circ(\text{Al}_{(s)}) + 3 \cdot \Delta H_f^\circ(\text{Cl}_{2(g)})] \\ &= [2 \cdot -45] - [2 \cdot 0 + 3 \cdot 0] = -90\text{KJ}\end{aligned}$$

Finally, for the last reaction:

$$\begin{aligned}\Delta H_R^\circ &= [2 \cdot \Delta H_f^\circ(\text{AlCl}_{3(s)})] - [3 \cdot \Delta H_f^\circ(\text{H}_{2(g)}) + \Delta H_f^\circ(\text{N}_{2(g)})] \\ &= [2 \cdot -705.63] - [3 \cdot 0 + 0] = -1411\text{KJ}\end{aligned}$$

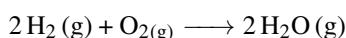
◆ STUDY CHECK

Using the enthalpy table, calculate ΔH_R° for the following reaction:



Answer: -25KJ .

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 related energy and the moles of reactants and products. For the exothermic reaction:



$\Delta H = -572\text{KJ}$.

the moles of hydrogen are related to heat as:

$$\frac{2 \text{ moles of H}_2}{-572 \text{ KJ}} \text{ or } \frac{-572 \text{ KJ}}{2 \text{ moles of H}_2}$$

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 reactant or products into heat.

Sample Problem 73

Hydrogen reacts with nitrogen to produce ammonia (NH₃) 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

$$5 \cancel{\text{ moles of NH}_3} \times \frac{-92 \text{ KJ}}{2 \cancel{\text{ moles of NH}_3}} = -230 \text{ KJ,}$$

that is: 5 moles of ammonia produce -230KJ. The fact that this value is negative means that heat will be released.

◆ STUDY CHECK

Calculate the number of hydrogen moles needed to generate -200KJ.

Answer: 6.5 moles.

7.5 Hess's Law: Manipulating reaction enthalpies

In the previous section we relied on a table of standard enthalpies of formation in order to compute enthalpy changes in general reaction. 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 on its natural state—and set up an equation that helps you find out the missing enthalpy.

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Reverting reactions Imagine they give you the following reaction:

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and you need to calculate the enthalpy change for this other reaction:



If you compare both reaction you will see the second reaction equals to 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:

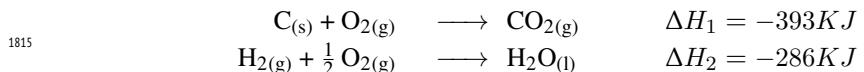


and you need to calculate the enthalpy change for this other reaction:

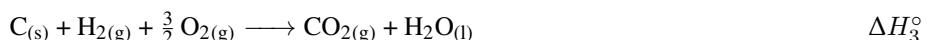


If you compare both reaction you will see the second reaction equals to the first reaction timed by two. If you time a reaction by two, the enthalpy change should also be timed by two. Therefore, $\Delta H_2^\circ = 2 \cdot -114 = -228 \text{KJ}$.

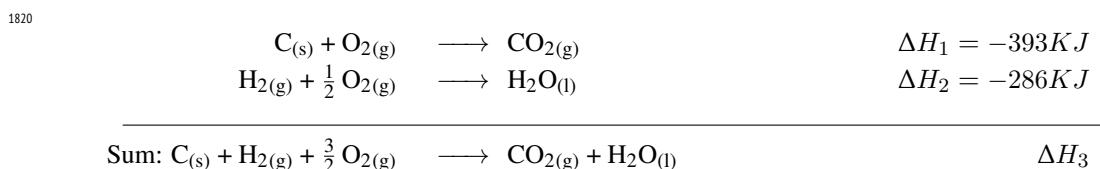
Combining reactions Imagine they give you the following two reactions:



and ask the enthalpy change for the following reaction:



If you look closely to the last reaction, you will see it results from adding the first two reactions, so that:



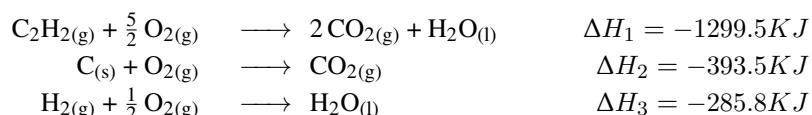
Therefore, $\Delta H_3 = \Delta H_1 + \Delta H_2 = -679 \text{KJ}$. When adding two chemical reactions the resulting enthalpy is the result of adding the enthalpy of both reactions.

Sample Problem 74

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

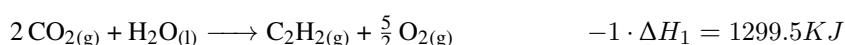
(1), (2) and (3), by adding, subtracting, or multiplying by a number so that the results adds up to reaction (4). A trick to do this is compare molecule by molecule in reaction (4) and see in which reaction we can find the same one. For example, reaction (4) contains $2C_{(s)}$ in the reactant side. $C_{(s)}$ can also be found in (2) also as reactant. However, in (2) $C_{(s)}$ is not timed by 2. There we will use two times reaction (2):



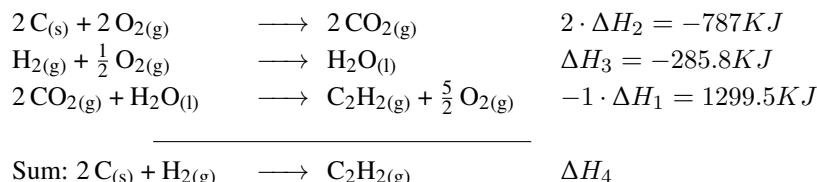
Reaction (4) also contains $H_{2(g)}$, which can be found in (3). There we will use (3) as it is:



Reaction (4) also contains $C_2H_{2(g)}$ 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:

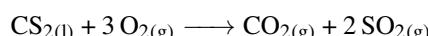


Therefore in the enthalpy for the reaction (4) will be:

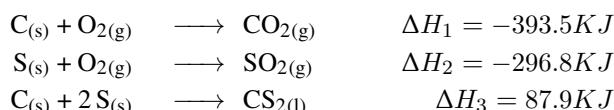
$$\Delta H_4^\circ = 2 \cdot \Delta H_2 + \Delta H_3 - 1 \cdot \Delta H_1 = 226.7 KJ$$

◆ STUDY CHECK

Calculate the enthalpy for this reaction:



Given the following thermochemical equations:



Answer: $-1075 KJ$.

Table 7.3 Standard enthalpy table at 1atm and 298K in KJ/mol.

Substance	ΔH_f°	Substance	ΔH_f°	Substance	ΔH_f°
Aluminum					
Al _(s)	0	AlCl _{3(s)}	-705.63	Al ₂ O _{3(s)}	-1675.5
Al(OH) _{3(s)}	-1277	Al ₂ (SO ₄) _{3(s)}	-3440	NH _{3(aq)}	-80.8
NH _{3(g)}	-46.1	NH ₄ NO _{3(s)}	-365.6	Al _(g)	314
Barium					
BaCl _{2(s)}	-858.6	BaCO _{3(s)}	-1213	Ba(OH) _{2(s)}	-944.7
BaO _(s)	-548.1	BaSO _{4(s)}	-1473.2	BaSO _{4(s)}	-1473.2
Boron					
BCl _{3(s)}	-402.96				
Bromine					
Br _{2(l)}	0	Br _{-(aq)}	-121	Br _(g)	111.884
Br _{2(g)}	30.91	BrF _{3(g)}	-255.60	HBr _(g)	-36.29
Cadmium					
Cd _(s)	0	CdO _(s)	-258	Cd(OH) _{2(s)}	-561
CdS _(s)	-162	CdSO _{4(s)}	-935		
Calcium					
Ca _(s)	0	Ca _(g)	178.2	Ca _(g) ²⁺	1925.90
CaC _{2(s)}	-59.8	CaCO _{3(s)}	-1206.9	CaCl _{2(s)}	-795.8
CaCl _{2(aq)}	-877.3	Ca ₃ (PO ₄) _{2(s)}	-4132	CaF _{2(s)}	-1219.6
CaH _{2(s)}	-186.2	Ca(OH) _{2(s)}	-986.09	Ca(OH) _{2(aq)}	-1002.82
CaO _(s)	-635.09	CaSO _{4(s)}	-1434.52	CaS _(s)	-482.4
CaSiO _{3(s)}	-1630				
Caesium					
Cs _(s)	0	Cs _(g)	76.50	Cs _(l)	2.09
Cs _(g) ⁺	457.964	CsCl _(s)	-443.04		
Carbon					
C _{graphite(s)}	0	C _{diamond(s)}	1.9	C _(g)	716.67
CO _{2(g)}	-393.509	CS _{2(l)}	89.41	CS _{2(g)}	116.7
CO _(g)	-110.525	COCl _{2(g)}	-218.8	CO _{2(aq)}	-419.26
HCO _{3^-(aq)}	-689.93	CO _{3^2-(aq)}	-675.23		
Chlorine					
Cl _(g)	121.7	Cl _{-(aq)}	-167.2	Cl _{2(g)}	0
Chromium					
Cr _(s)	0				
Copper					
Cu _(s)	0	CuO _(s)	-155.2	CuSO _{4(aq)}	-769.98
Fluorine					
F _{2(g)}	0				
Hydrogen					
H _(g)	218	H _{2(g)}	0	H _{2O(g)}	-241.818
H _{2O(l)}	-285.8	H _{+(aq)}	0	OH _{-(aq)}	-230
H _{2O₂}	-187.8	H ₃ PO _{4(l)}	-1288	HCN _(g)	130.5
HBr _(l)	-36.3	HCl _(g)	-92.30	HCl _(aq)	-167.2
HF _(g)	-273.3	HI _(g)	26.5		
Iodine					
I _{2(s)}	0	I _{2(g)}	62.438	I _{2(aq)}	23
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 the chemical bonds of a carbohydrate molecule? (c) What is the name of the energy stored in height?

7.2 Carry the following conversions: (a) 650J into calories (b) 3.25 kcal into joules (c) 41°F into celsius

7.3 Carry the following conversions: (a) 20°C to F (b) 300K to °C

THE FIRST LAW OF THERMODYNAMICS

7.4 A sample of gas expands from 3 to 4 L at constant pressure. Using $1L \cdot atm = 101.3J$, 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

7.5 A 50g piece of aluminum ($c_e = 0.214 \frac{cal}{g^\circ C}$) initially at 25°C absorbs 100cal. Calculate the final temperature of the aluminum piece.

7.6 A sample of gas expands carrying work on the surroundings of 120J and absorbing 150J of heat from the surroundings. Calculate the change of the internal energy of the system in J.

7.7 A 200g piece of iron ($c_e = 0.1 \frac{cal}{g^\circ C}$) initially at 15°C absorbs 1000cal. Calculate the final temperature of the metal piece.

7.8 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 $0.108 \frac{cal}{g^\circ C}$.

7.9 What is the final temperature of a 35 g sample of iron at 25°C after receiving 50cal? Iron has a specific heat of $0.108 \frac{cal}{g^\circ C}$.

7.10 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 $0.2 \frac{cal}{g^\circ C}$.

7.11 What is the specific heat of a metal if a 100 g sample at 25°C warms up until 50°C after receiving 100cal?

CALORIMETRY

7.12 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.

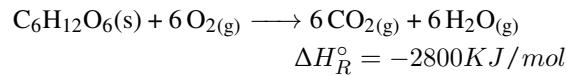
7.13 A 10 grams sample of fructose (MW=180g/mol) is burned in a constant-volume calorimeter containing 50g of water. The temperature inside the calorimeter increases 7°C . The calorimeter constant is $10.8 \frac{kJ}{^\circ C}$. Calculate the molar heat of the reaction.

7.14 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.

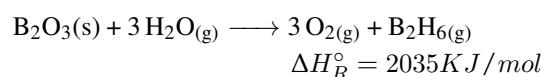
7.15 We mix 50mL of 2M HCl with 100mL of 1.5M NaOH in a coffee-cup calorimeter. Both solutions are initially at 20°C. Calculate the final temperature of the solution in the calorimeter considering that the specific heat of the mixture is $4.184 \frac{J}{g^\circ C}$ and the density of the solution is 1g/mL. The molar heat of the reaction is -56kJ/mol.

ENTHALPY

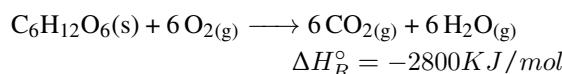
7.16 Identify the following reaction as endothermic or exothermic.



7.17 Identify the following reaction as endothermic or exothermic.



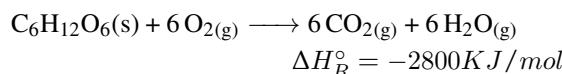
7.18 For the following reaction:



Fill the conversion factor:

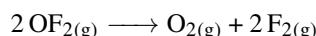
$$\frac{\text{moles of O}_2}{-2800 \text{ KJ}}$$

7.19 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.

7.20 Calculate the enthalpy of reaction for:



given:

$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 24.5 \text{ KJ}$$

7.21 Calculate the enthalpy of reaction for:



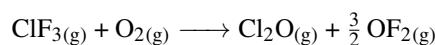
given:

$$\Delta H_f^\circ(\text{ClF}_{(\text{g})}) = -56 \text{ KJ}$$

$$\Delta H_f^\circ(\text{Cl}_2\text{O}_{(\text{g})}) = 88 \text{ KJ}$$

$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 25 \text{ KJ}$$

7.22 Calculate the enthalpy of reaction for:



given:

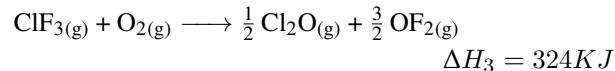
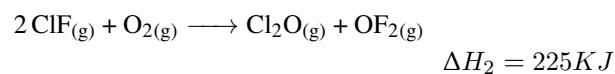
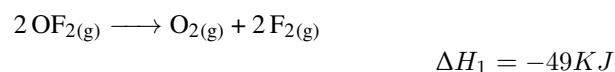
$$\Delta H_f^\circ(\text{ClF}_{3(\text{g})}) = -156 \text{ KJ}$$

$$\Delta H_f^\circ(\text{Cl}_2\text{O}_{(\text{g})}) = 88 \text{ KJ}$$

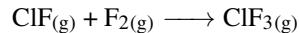
$$\Delta H_f^\circ(\text{OF}_{2(\text{g})}) = 25 \text{ KJ}$$

HESS'S LAW

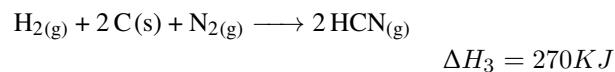
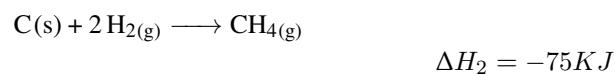
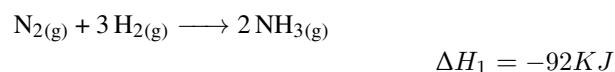
7.23 Using the following reactions:



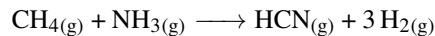
Determine the enthalpy change for:



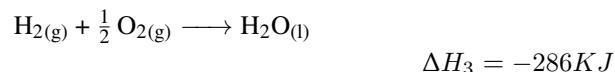
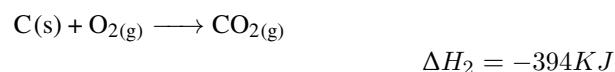
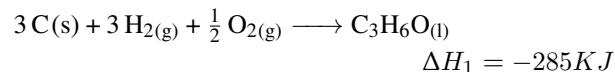
7.24 Using the following reactions:



Determine the enthalpy change for:



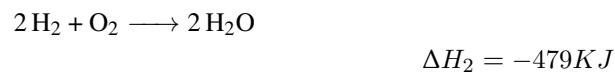
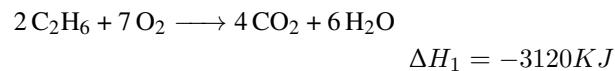
7.25 Using the following reactions:



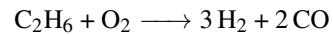
Determine the enthalpy change for:



7.26 Using the following reactions:



Determine the enthalpy change for:



Answers **7.1** (a) kinetic energy (b) chemical energy (c) potential energy **7.3** (a) $68^{\circ}F$ (b) $27^{\circ}C$ **7.5** $34.34^{\circ}C$
7.7 $T_{Final} = 65^{\circ}C$ **7.9** $38^{\circ}C$ **7.11** $0.04\text{cal/g}^{\circ}\text{C}$ **7.13** -1387KJ/mol **7.15** $29^{\circ}C$ **7.17** endothermic **7.19** 8400KJ
7.21 225KJ **7.23** -187KJ **7.25** -1755KJ

8

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 other—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 from 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 by means of stronger force that act between molecules—these are called intermolecular forces. The properties of these forces will help you understand why some liquids boil at higher temperature than others or some solids have higher melting point.



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GOALS

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- 1 Identify intermolecular forces
- 2 Identify different types of solids
- 3 Identify units cells
- 4 Calculate density of solids
- 5 Calculate vapor pressure

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8.1 Intermolecular forces

Atoms in liquid or solid compound are connected by means of 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 by means of intermolecular forces. The word intermolecular means between molecules. This section describes the three existing types of intermolecular forces as well as its nature and intensity.

Discussion: Do you know other states of the matter other than solid, liquid, or gas?

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Intermolecular forces and intramolecular interactions

Molecules are made of atoms which connect by means of *intramolecular* interactions such as covalent or ionic bonds. Differently, molecules interact with each other by means of *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 in order to melt or boil a chemical we need to overcome the intermolecular forces that connect molecules in order 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).

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Dispersion forces All molecules are made of atoms which contain electrons. The

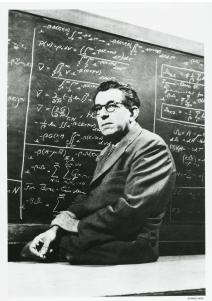
▼ Polymer molecules interact by means of dispersion



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▼ Fritz London a german physicist is responsible for the name of London forces



1868

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▼ geckos stick because of the van der Waals force



1870

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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 dipoles are responsible for London dispersion forces, also called Van der Waals forces or simply dispersion forces.

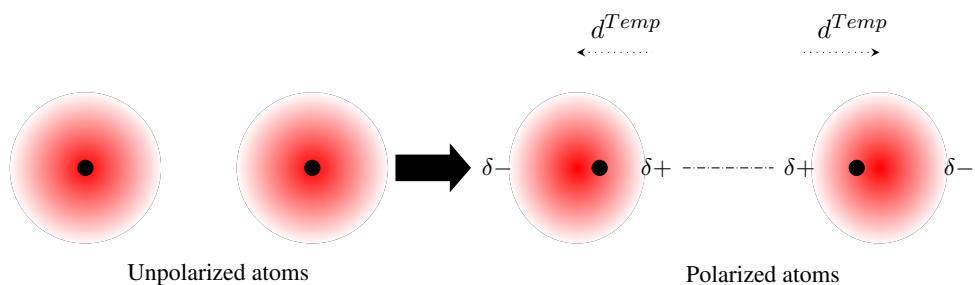


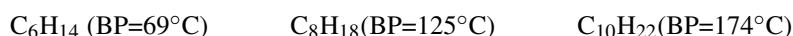
Figure 8.1 Dispersion forces result from instantaneous dipole moments resulting from the polarization of the electron density of atoms and molecules.

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. 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.

Table 8.1 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

The melting (or freezing) and boiling point of the noble gases are given in Table 8.1, 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 point 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:



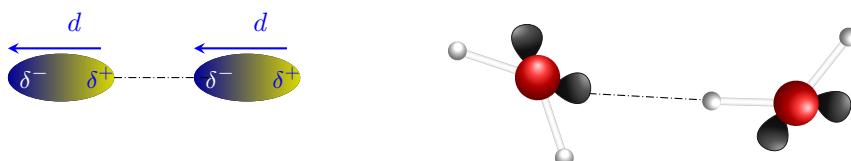
Dipole-Dipole forces Atoms have different electronegativity that is, a different tendency to attract the electron density in a bond. In the periodic table, electronegativity increases going from left to right and top to bottom. Elements in the top right of the table (Cl, F) tend to be very electronegative and hence they tend to strongly attract the electrons on a 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 moments result from differences in electronegativity. When an electronegative atom is

1890 connected to a electropositive atom in a bond, the electronegativity difference creates permanent dipole moments and molecules with permanent dipole moment 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 results from the combination of a 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. This types of interactions are stronger than dispersion forces but weaker than normal interatomic covalent bonds. Molecules with dipole moment can attract each other by means of dipole forces, orienting themselves so that their positive side aligns with the negative side maximizing the electrostatic attraction. At the same type, dipole forces depend on the distance and at large distance are less effective.

1900



1905

Figure 8.2 (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

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 a almost null dipole moment, whereas the later 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 list some dipole moments and boiling points showing the trend that the larger the dipole moment the higher (more positive) the boiling point.

1910

Table 8.2 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 molecule with hydrogen bonds are HF or NH₃. Hydrogen bonds are a specific type dipole-dipole interactions responsible, among other, for some of

1915

the high boiling point 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 bond possible.

1920

Sample Problem 75

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 .

Answer: all have dispersion, only NH_3 , HF has dipole and only NH_3 , HF has H-bonds.

1930 *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. In order 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 by means of weak dispersion forces. Imagine now boiling water. Water is polar and water has O–H bonds, hence water molecules interact by means of 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.

1935

1940

Sample Problem 76

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.

Answer: BP(CH₃F) > BP(CH₄).

8.2 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.

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.

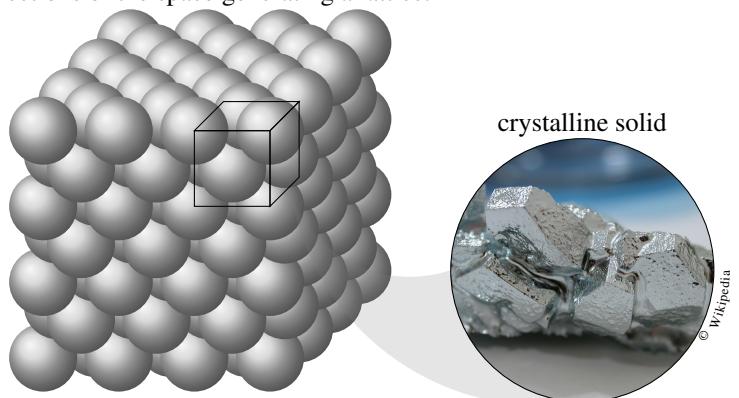


Figure 8.3 Unit cell of a solid of a crystalline solid. The whole structure of the solid results from the replication of a unit cell and just this unit cell is necessary to characterize the structure of the solid.

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 tree 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, CaF₂. 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 ($\text{Au}_{(s)}$).

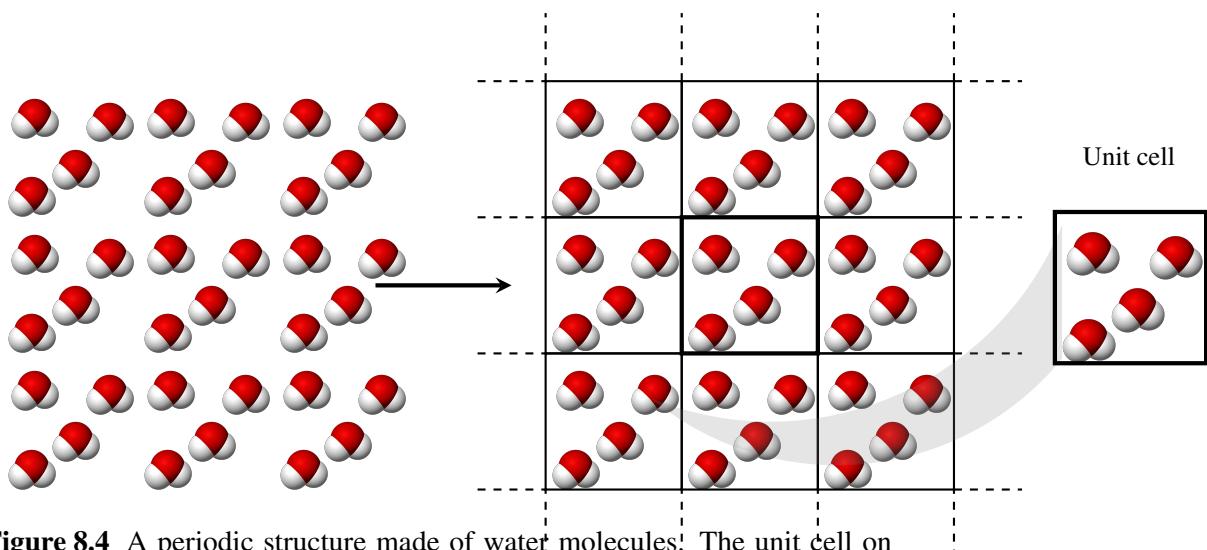


Figure 8.4 A periodic structure made of water molecules. The unit cell on the left contains four water molecules. The repetition of the unit cell, on the right, generates a two-dimensional structure.

Sample Problem 77

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 an 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 $\text{NH}_3(s)$.

Answer: metallic, atomic, ionic and molecular.

8.3 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.

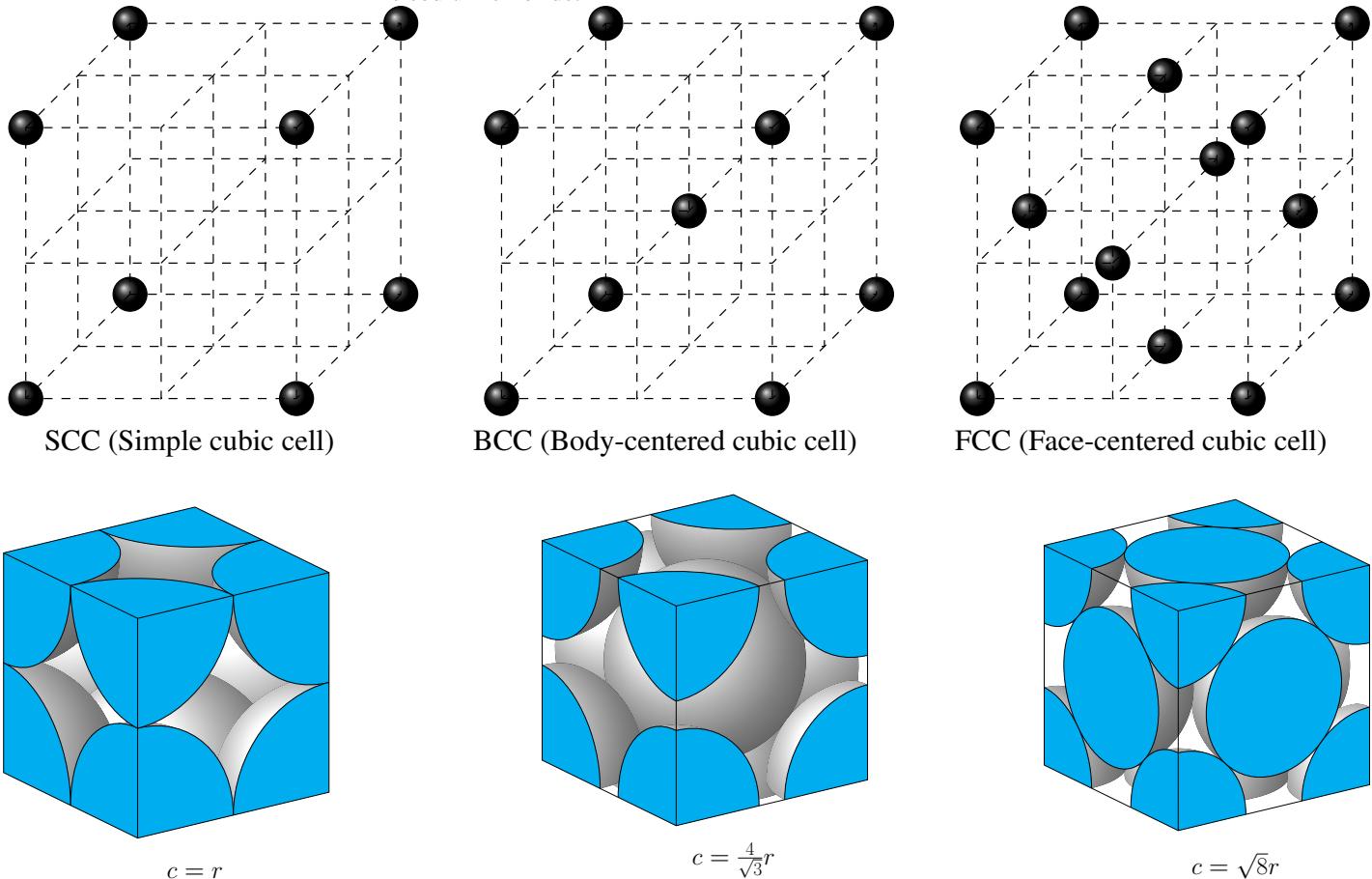


Figure 8.5 The different unit cells. Space-fill structures are shown on the bottom. The simple cubic unit cells have atoms in the corners of the cell. The body-centered cubic unit cell have atoms in the corners and one atom in the center. The face-centered unit cell has atoms in the corners and in the faces. The relationship between the cell parameter (c) and the atomic radius (r) is also given for each unit cell.

1985 *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).

2000 Atom sharing in unit cells Before we cover the different metallic units cells let us talk about atom sharing. Think about a cubit 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 corders. 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.

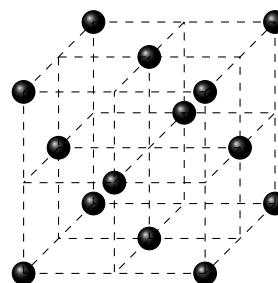
2005

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Sample Problem 78

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

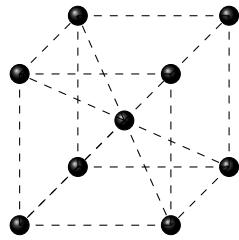
If you count the number of spheres in the drawing you might think the cell contains fourteen atoms. However, this is not true, as each sphere is shared by other unit cells. Remember each location of the unit cell counts as a fraction. If an atom is fully inside in the cell—not in the vertexes, neither in the faces or sides—the sharing factor is one. If an atom belongs to a vertex, the sharing factor is $\frac{1}{8}$. Atoms in a face has a sharing factor of $\frac{1}{2}$ and atoms in the edges have a sharing factor of $\frac{1}{4}$.

Location	Sharing Factor, f	# atoms, N	$f \times N$
Corner	$\frac{1}{8}$	8	1
Faces	$\frac{1}{2}$	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:

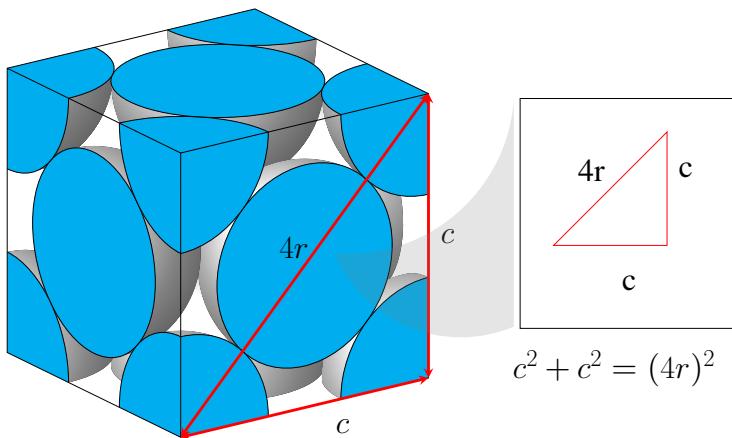


Answer: 2.

Metal unit cells Here we will cover three different metal unit cells, all cubic cells.

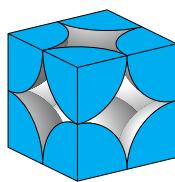
First, the simple cubic unit cell, with an atom each of the vertexes of the cell. This is the less compact unit cell with one atom per unit cell. Second, the body-centered unit cell is a cubic unit cell with atoms in the vertex of the cell and a single atom in the center of the cell. This cell has two 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 79

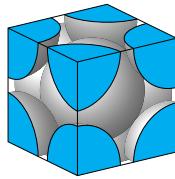
For the following unit cell, calculate the relationship between the cell parameter and the atomic radius.

**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.



$$\text{Answer: } c = \frac{4}{\sqrt{3}}r.$$

2040

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

2045

c is the cell parameter in pm

Sample Problem 80

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

2045

with cell parameter is 406pm.

Answer: $19.54 \text{ g} \cdot \text{ml}^{-1}$.

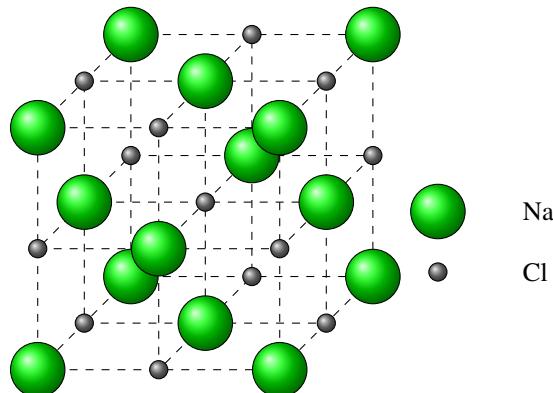
2050

2055

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 81

Calculate the formula for the following unit cell



SOLUTION

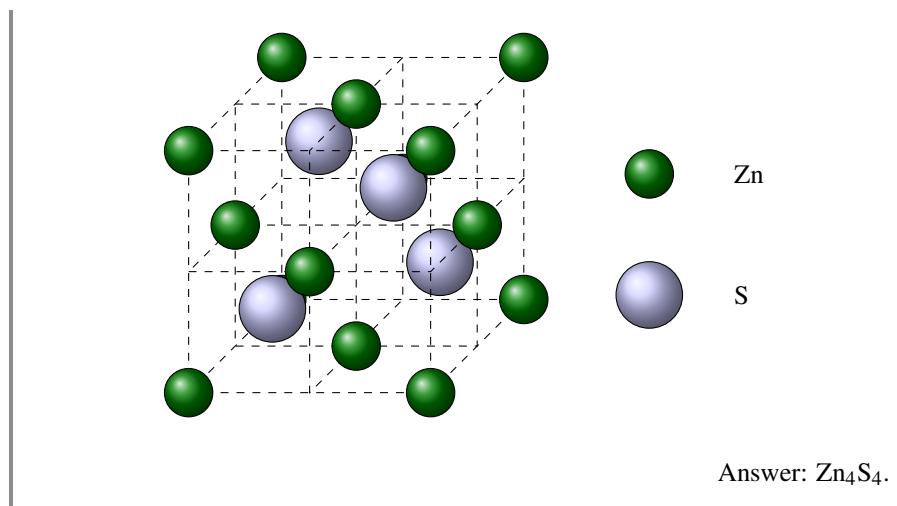
The unit cell contains Cl^- and Na^+ . Remember every location in the unit cell has different sharing factor. We will compute the number of atoms in each location and multiply by the sharing factor to calculate the number of Cl and Na in the cell:

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:



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.

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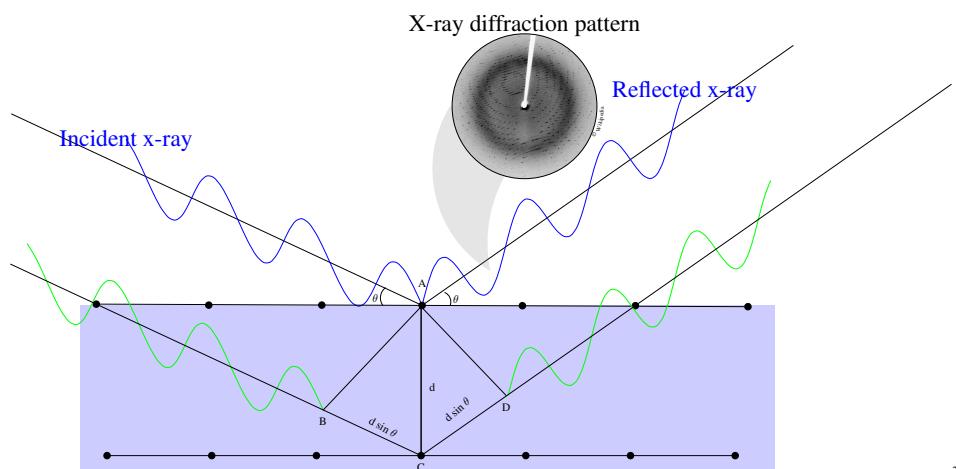


Figure 8.6 Reflection of x-rays in two different lattice points separated by a distance. The incident waves are in phase—maximums and minimums overlap—but the reflected waves are only in phase when the difference of distances traveled by both is an integral number of wavelengths. In the image $BC + CD = 2d \sin \theta$.

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 ($n=0, 1, 2, \dots$).

$$n\lambda = 2ds \sin \theta \quad (8.1)$$

Sample Problem 82

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.

Answer: 53°

8.4 Liquid state

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.

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 pulled in all directions by the intermolecular forces so that overall there is no net pull in any direction. The molecules at the surface are pulled down and to the side by the surrounding molecules. However, they are not pulled up and hence they experience a new pull inward that causes 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 the elastic force in the surface of the liquid. It is defined as the amount of energy needed to modify the surface of a liquid by unit of area, with units of milli Newton per meter, mN/m.

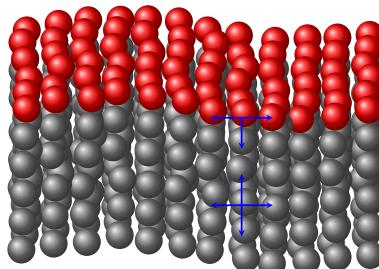


Figure 8.7 A representation of surface (red spheres) and bulk (blue spheres) liquid molecules as well as two types of meniscus: a concave and a convex meniscus, typical of water and mercury respectively. Surface molecules are pulled inwards creating the surface tension whereas bulk molecules are not.

Surface tension values depend on the temperature and the phases in contact and for example the surface tension of the water-air interface is different than the value for the water-mercury interface. The stronger the intermolecular forces, the higher the surface energy—it would take more energy to modify the surface of the liquid. For example, the surface tension of the C_6H_6 -air interface (29mN/m) is smaller than the surface tension of the H_2O -air interface (73mN/m). The surface tension is responsible for phenomena such as the beading of water on the plants 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. Capillary results from the competitive effect of cohesive and adhesive forces. In the case of mercury, the cohesive forces are stronger than the adhesive and the meniscus created is convex. In the case of water the adhesive forces are stronger and the meniscus is concave.

▼A paper clip standing on water



© wikipedia

▼Water droplets



© www.piclist.com

▼Meniscus of water and mercury



© Flickr

▼A viscous liquid



© Flickr

▼Capillary for tubes of different diameters



© wikipedia

Table 8.3 Surface tension (γ_t) values for several interfaces at different temperatures.

Interface	γ_t (mN/m)	T	Interface	γ_t (mN/m)	T
H_2O -Air	73	20°C	H_2O -Hg	415	20°C
CH_3I -Air	67	20°C	H_2O -Air	73	22°C
C_6H_6 -Air	30	20°C	H_2O -Air	72	25°C
CH_3OH -Air	22	20°C	Hg-Air	486	20°C

2105

▼ Rubbing alcohol has low heat of vaporization



2110

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2115

▼ Acetone has low heat of vaporization



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▼ Perfumes have low vaporization heat



© Wikipedia

2120

▼ Metals have high vaporization heat

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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 8.4 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 8.5 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

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

2135

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.

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Table 8.6 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

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.

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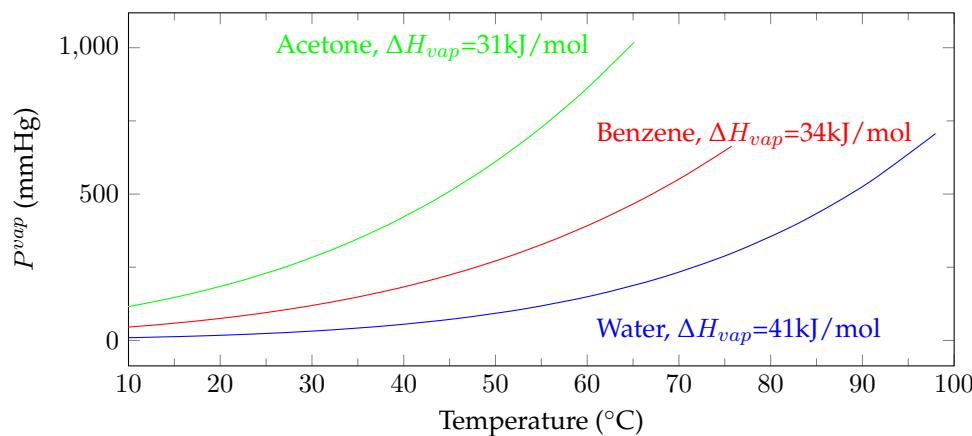


Figure 8.8 Vapor pressure change with temperature for three chemicals with different heat of vaporization.

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 to pairs of temperatures and hence two pairs of vapor pressures:

2160

$$\ln\left(\frac{P_{T_1}^{vap}}{P_{T_2}^{vap}}\right) = \frac{\Delta H_{vap}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Clausius-Clapeyron relation

where:

2165

$P_{T_1}^{vap}$ 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

Sample Problem 83

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 $P_{T_1}^{vap} = 0.03 atm$ and $T_2 = 323K$ and $P_{T_2}^{vap} = x$. We also have the enthalpy of vaporization. Mind 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

Answer: 97.80 J/mol.

8.5 Phase diagrams

2170 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.

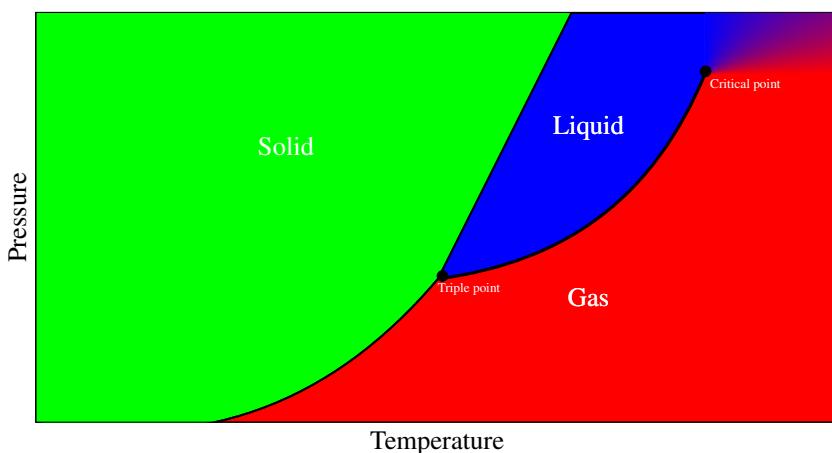
2175

Figure 8.9 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.

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

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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 1 atm, 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:

2210	Liquid \longrightarrow Solid	Freezing
	Liquid \longrightarrow Gas	Evaporation or vaporization
	Solid \longrightarrow Liquid	Melting
	Gas \longrightarrow Liquid	Condensation
2215	Solid \longrightarrow Gas	Sublimation
	Gas or Solid \longrightarrow Liquid	Liquefy

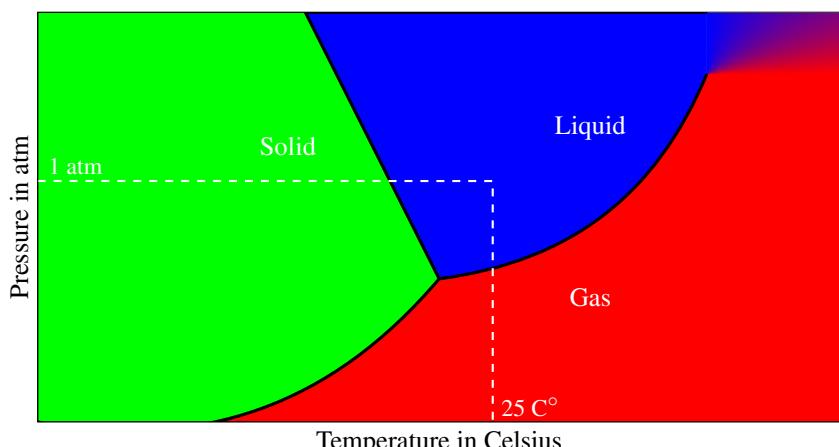


Figure 8.10 The phase diagram of water with pressure in the Y axis and temperature in the X axis. This diagram displays the different states of matter of water for different pressure and temperature conditions. The coordinates of the triple point are $(0.0098\text{ C}^\circ, 0.0060\text{ atm})$. This 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 $(\text{Temperature}, \text{Pressure})$ 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.

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.

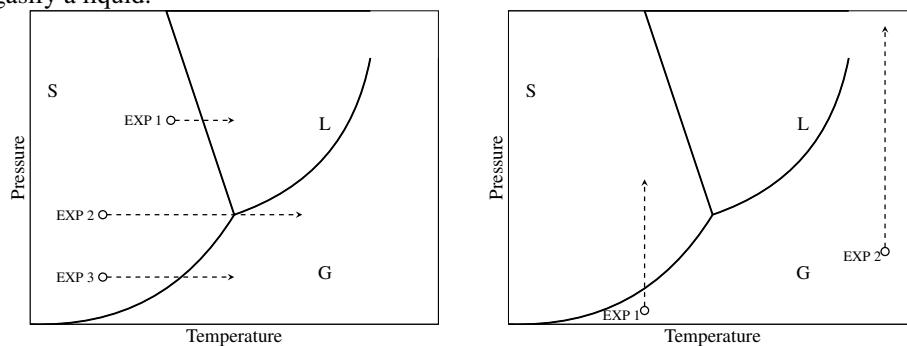


Figure 8.11 Heating experiments (left) and compression experiments (right).

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:

$$Q = m \cdot c_e^{\text{H}_2\text{O}(\ell)} \cdot \Delta T_1 + n \cdot \Delta H_{\text{vap}}^{\text{H}_2\text{O}} + m \cdot c_e^{\text{H}_2\text{O(g)}} \cdot \Delta T_2$$

Table 8.7 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	

CHAPTER 8

INTERMOLECULAR FORCES

8.1 Indicate the strongest intermolecular force existing between the molecules of the following compounds:
 (a) CH₃OH (b) H₂ (c) CCl₄

8.2 Indicate the strongest intermolecular force existing between the molecules of the following compounds:
 (a) CH₄ (b) CCl₃H (c) HF (d) HCl

8.3 From the following pair of molecules, which molecule forms intermolecular H bonds? (a) HF or H₂
 (b) NH₃ or CH₄

8.4 From the following pair of molecules, which molecule forms intermolecular H bonds?
 (a) CH₃—O—CH₃ or H₂O (b) HCl or HF

8.5 From the following pair of molecules, which molecule forms stronger dispersion forces? (a) Ar or He (b) H₂O or H₂S

8.6 From the following pair of molecules, which molecule forms stronger dispersion forces? (a) CH₃CH₃ or CH₄ (b) CH₄ or CH₃Cl

8.7 From the following pair of molecules, which molecule forms stronger dipole forces? (a) HCl or HBr
 (b) H₂O or H₂S

8.8 From the following pair of molecules, which molecule forms stronger dipole forces? (a) NH₃ or H₂O
 (b) HI or HBr

8.9 From the following pair of molecules, which molecule has higher boiling point? (a) CH₃CH₃ or CH₄
 (b) CO₂ or H₂O

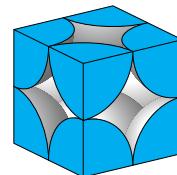
8.10 From the following pair of molecules, which molecule has higher boiling point? (a) HF or HCl (b) Ar or He

THE SOLID STATE

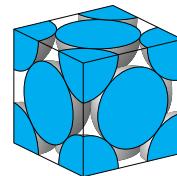
8.11 Indicate the number of atoms contained in the body-centered (bcc) cubic unit cell, for structures with the same type of atoms.

8.12 Indicate the number of atoms contained in the simple cubic (sc) unit cell, for structures with the same type of atoms?

8.13 The image displays the structure of Polonium. What is the number of atoms per unit cell for this metal?



8.14 The image displays the structure of Gold. What is the number of atoms per unit cell for this metal?

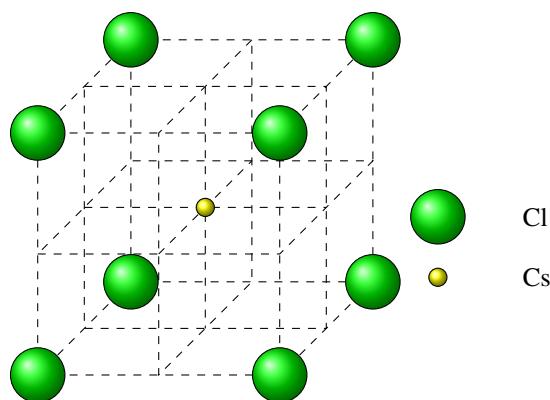


8.15 Identify the type of crystalline solid formed by the following compounds: (a) cesium chloride (b) tungsten

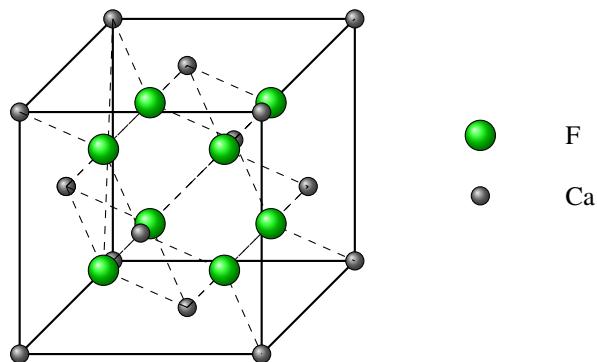
8.16 Identify the type of crystalline solid formed by the following compounds: (a) acetic acid (b) hydrogen sulfide

8.17 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.

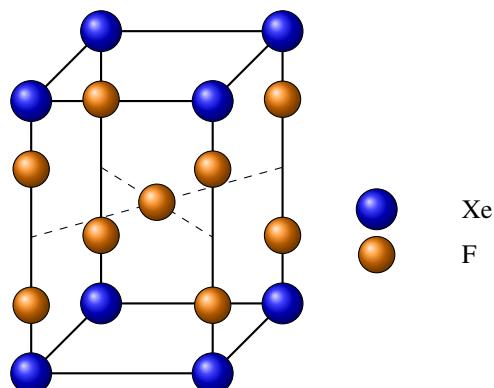
8.18 Calculate the formula for the following unit cell:



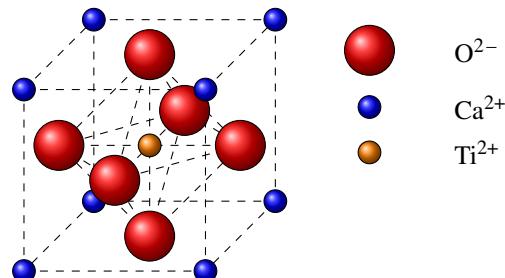
8.19 Calculate the formula for the following unit cell:



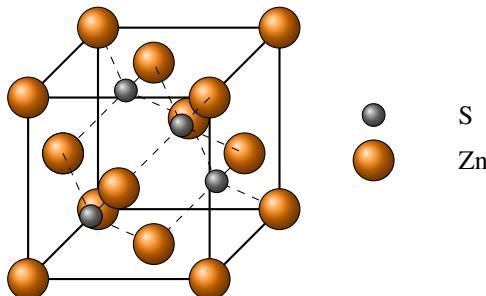
8.20 Calculate the formula for the following unit cell:



8.21 Calculate the formula for the following unit cell:

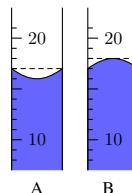


8.22 Calculate the formula for the following unit cell:

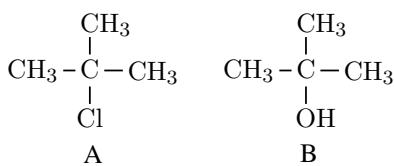


LIQUID STATE

8.23 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)



8.24 Which of the following molecules present higher viscosity?



8.25 A liquid has an 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.

8.26 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?

8.27 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.

8.28 Calculate the heat of vaporization of a chemical that doubles its vapor pressure when the temperature increases from 10°C to 40°C.

8.29 For a chemical with heat of vaporization of 200kJ/mol, at what temperature will the vapor pressure be three times the value at 25°C?

8.30 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.

8.31 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 ($\Delta H_{vap}=15\text{ kJ/mol}$)

8.32 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 ($\Delta H_{vap}=41\text{ kJ/mol}$)

Answers 8.1 (a) CH₃OH (hydrogen bonds) (b) H₂ (dispersion forces) (c) CCl₄ (dispersion forces) **8.3** (a) HF (b) NH₃ **8.5** (a) He (b) H₂S **8.7** (a) HCl (b) H₂O **8.9** (a) CH₃CH₃ (b) H₂O **8.11** 2 **8.13** 1 **8.15** (a) cesium chloride (ionic solid) (b) tungsten (atomic solid, metallic) **8.17** 20 g · mol⁻¹ **8.19** Cs₁Cl₁ **8.21** Cs₁Cl₁ **8.23** (a) a: concave; b: convex (b) b (c) a **8.25** 4.51atm **8.27** 1.52atm **8.29** 303°C

PART

ONE

9

Electronic structure of atoms

MATTER is everywhere around you, from the water you drink to the air you inhale. 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 than 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.



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9.1 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, or 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. 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 vacuum.

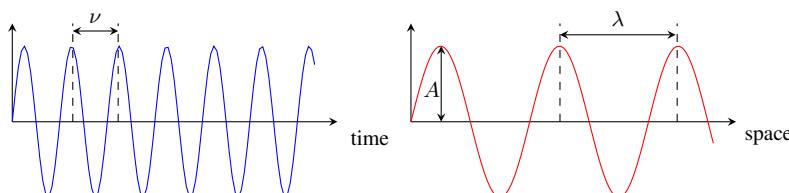


Figure 9.1 Properties of waves. Waves are characterized by its frequency, wavelength and amplitude and in the vacuum they travel at the speed of light.

Frequency and energy Light travels in time. That is the reason you can hear a whistle from afar. The *frequency* of a radiation—the frequency of a specific type of

GOALS

- 1 Compute frequency, wavelength and the energy of light
- 2 Compute Hydrogen energy levels
- 3 Compute Hydrogen transition energies
- 4 Obtain electronic configurations
- 5 Compare periodic properties

2265

Discussion: Look around your apartment and find four different types of radiation.

2270

“ The present is the only thing that has no end.
Schrödinger **”**

light—characterizes how this radiation oscillates in time. The unit of frequency is the hertz and frequency is represented by the symbol ν . At the same time, frequency is connected to the energy of radiation. High frequency radiation are very energetic. Think for example of gamma rays; these type of radiation produced in 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

2275

$h = 6.6 \times 10^{-34}$ is called Plank's constant

ν is frequency in hertz ($\text{Hz}=\text{s}^{-1}$)

2280

As you can see in the previous formula, the frequency is directly proportional to 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 color. The radiation emitted changes as the body is 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 phenomena. Plank came with a solution for the dilemma. Classical physics assumes that radiant energy is a continuous and radiation can be emitted and absorbed at any amount. In order 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 to $h\nu$, 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 solve the blackbody radiation dilemma and change physics forever, marking the beginning of a new quantum theory.

2285

2290

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 water or 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: the frequency and its wavelength:

$$c = \nu \cdot \lambda \quad \text{the speed of light}$$

where:

2295

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:

2500

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. 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 in the surface in water. The energy of light also propagates in space and the *wavelength* of a radiation is the distance between two consecutive peaks. As such, wavelength, represented by the letter λ and with units of nm is also related to energy by means of the formula:

$$E = \frac{1.98 \times 10^{-16}}{\lambda}$$

wavelength formula

where:

E is the energy in joules

2305

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.

2310

Sample Problem 84

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 wavelength 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:

$$\nu = \frac{3 \times 10^{17}}{\lambda} = \frac{3 \times 10^{17}}{300} = 1 \times 10^{15} \text{ Hz}$$

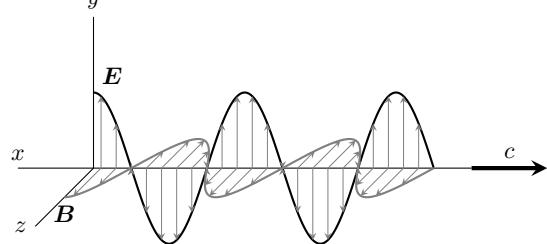
❖ STUDY CHECK

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 $2 \times 10^{15} \text{ Hz}$.

Answer: (a) 353nm ; (b) $7.2 \times 10^{10}\text{Hz}$; (c) $4.1 \times 10^6\text{nm}$

2315

The electromagnetic spectrum of light Visible light consist of electromagnetic waves, which have an electric field and magnetic field component. These two components share the same wavelength, frequency, and speed but are perpendicular to each other.



2320

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 slit a bright spot is generates on the other side of the slit. When a source of light passes through two slits surprising results arise.

2325

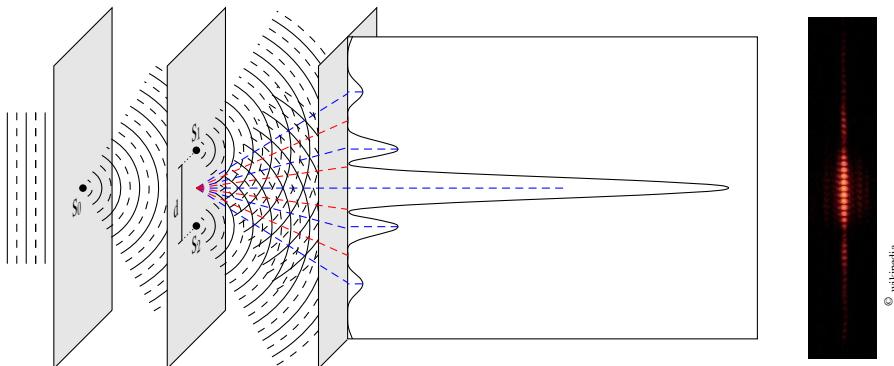


Figure 9.3 The double-slit experiment demonstrating the wave nature of light. Using one slit leads to a single bright spot. Using two slits leads to a set of patterns of light and darkness resulting from the interference of light. Red lines represent destructive interference whereas blue lines represent constructive interferences.

2330

One would expect to see two bright spots, one per each slit. However, what you really would see would be a series of bright spots and dark spots, resulting of the interference of light. As light is a wave it can interfere and light plus light does not always gives more light, and can sometimes genera 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.

▼Standing waves of a guitar



© wikipedia



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▼Traveling waves

▼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. For example, radiation with wavelength of 10^{-2} nm belongs to gamma rays radiation, whereas radiation with 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.

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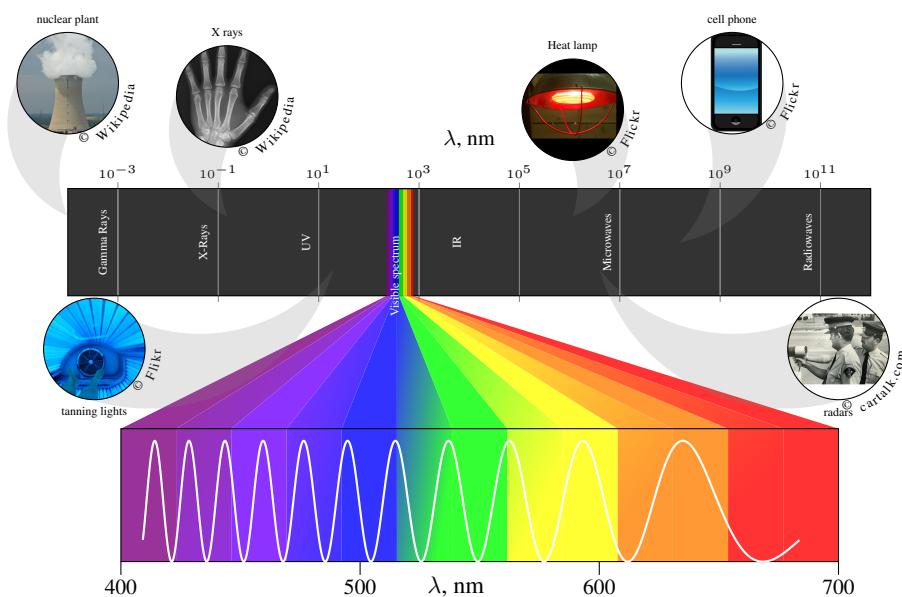


Figure 9.4 Spectrum of the electromagnetic radiation, from gamma rays (shortest wavelength) to radio waves (highest wavelength). The visible part of the spectrum ranges from 400 nm (violet) to 700 nm (red).

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Light not always have color. Only a small range of wavelengths belong to visible radiation and the visible spectrum correspond 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 $\lambda = 450$ nm will be blue light. Ultraviolet radiation is the most energetic visible radiation whereas infra red waves are the less energetic waves of the visible spectrum.

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Table ?? 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
IR	$4 \times 10^{14} - 4 \times 10^{11}$	Green	500-565
MicroW	$3 \times 10^{11} - 3 \times 10^8$	Yellow	565-590
RadioW	$3 \times 10^8 - 3 \times 10^3$	Orange	590-625
		Red	625-740

Sample Problem 85

Indicate: (a) the color of a radiation with $\lambda = 650\text{nm}$; (b) the type of a radiation with $\lambda = 10^5\text{ nm}$; (c) the type of a radiation with $\nu = 10^{16}\text{ Hz}$.

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. Finally, in order to answer the last question we need to convert frequency into wavelength, as the figure above only indicates wavelength. $\nu = 10^{16}\text{ Hz}$ corresponds to $\lambda = 30\text{ nm}$. Hence, this frequency corresponds to the UV.

◆ STUDY CHECK

Indicate: (a) the color of a radiation with $\nu = 7.5 \times 10^{14}\text{ Hz}$; (b) the type of a radiation with $\nu = 10^8\text{ Hz}$.

Answer: (a) violet; (b) Microwaves.

Electron-Volt a new unit of energy Sometimes, it is convenient to use another energy unit, called electron-volt, that makes these values have more reasonable values.

$$1\text{eV} = 1.60218 \times 10^{-19}\text{ J} \quad \text{or} \quad \frac{1\text{eV}}{1.60218 \times 10^{-19}\text{ J}}$$

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 $E_3 = -1.5\text{J}$. 2350

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The photoelectric effect The photoelectric effect was a mysterious phenomena discovered early in the twentieth century. Scientist found that if you expose a metal to light, under certain conditions, it emits electrons—it produced electricity. They found that the intensity—the brightness—of the radiation was not a key component of this phenomena, and not by increasing the intensity you were able to produce electrons.

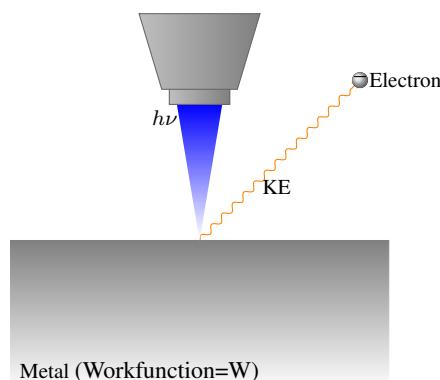


Figure 9.5 The photoelectric effect: when light with frequency (ν) larger than a threshold irradiates a metal, electrons are ejected with a specific kinetic energy (KE) that depends on the work function (W) of the metal.

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They 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. On that time, the current theory of light, associating intensity of light with

energy, was unable to explain this phenomena. Albert Einstein used Plank's theory of the blackbody radiation to solve this mystery. He assumed that light is made of a 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.

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Table 9.2 List of metal 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}

In Table 9.2 you can find numerous workfunctions. Metals such as Fe have high workfunctions in comparison to metals such as Ca, that means it takes more energy to remove an electron from the metal. Therefore, if the energy of the radiation was enough to overcome this forces, the 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:

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$$KE = 4.13 \times 10^{-15} \nu - W \quad \text{Photoelectric effect}$$

where:

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KE is the kinetic energy of the emitted electrons in eV

4.13×10^{-15} is called Plank's constant in $\text{eV} \cdot \text{s}$, h

ν is frequency in hertz (Hz)

is the workfunction 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 $\text{eV} \cdot \text{s}$, h , ν_c is the threshold frequency in hertz (Hz) and W is the workfunction of the metal in eV. Einsteins theory of the photoelectric effect shocked the scientific community. Before this theory, light was considered a wave. Based on Einstein's theory, wave poses properties of both a particle and a wave, and depending on the experiment one experience light as a wave or as a particle.

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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

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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

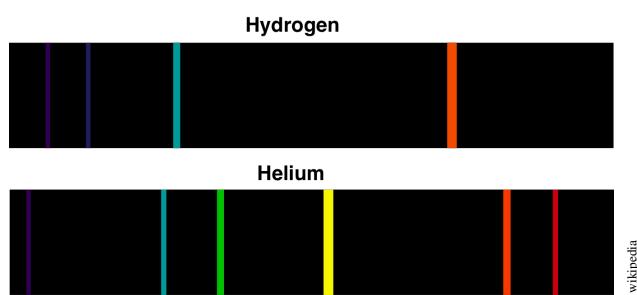
A metal with workfunction of 5eV is exposed to a radiation source with frequency of $9 \times 10^{14}\text{Hz}$. Indicate whether electrons will be ejected and if so, indicate the kinetic energy of these.

Answer: no electrons will be ejected

9.2 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 in which an atom absorbs or emits radiation. Each atoms has a distinctive emission spectrum. Some of these lines correspond to the visible spectrum, that is, they can be seen. Others correspond higher or lower parts of the spectrum. This section will cover the spectrum of hydrogen.



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Figure 9.6 Atomic spectrum of two atoms showing the lines corresponding to the visible.

Atomic line spectrum of hydrogen Newton shown that sunlight (white light) is composed of various components of different colors. 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.

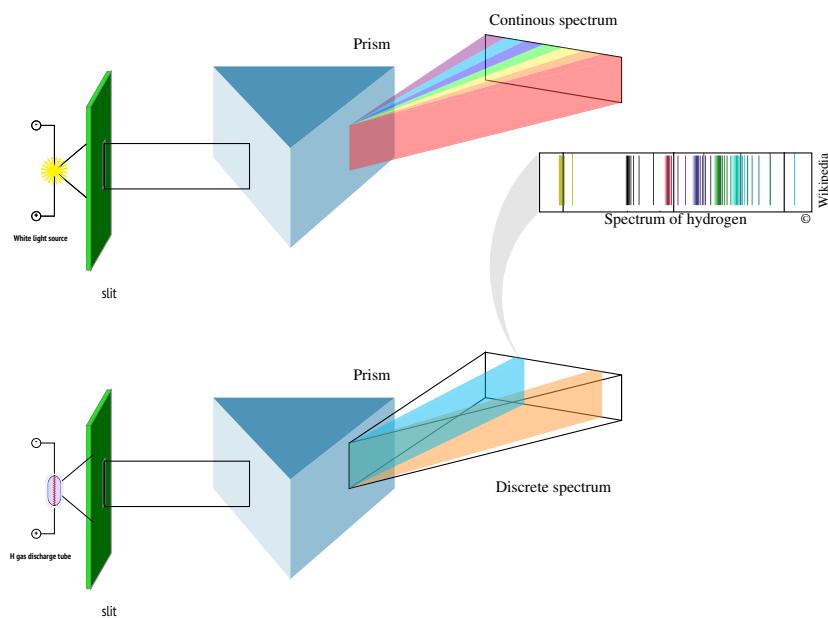


Figure 9.7 The spectrum of hydrogen: white light contains radiation of all colors of the visible spectrum whereas light coming from hydrogen contains a quantized series of lines.

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The atomic line spectrum presents of a gas is a set of lines on a black (or sometimes white) background. These lines correspond to radiation emitted (or absorbed) by atoms. 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.

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The Bohr 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:

$$E_n = -2.178 \times 10^{-18} \frac{1}{n^2}$$

Bohr formula in J

where:

E_n is the energy of the level n in joules

n is the number of the level

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$-2.178 \times 10^{-18} \text{ J} = R_H$ is called the Rydberg constant (-13.59 eV)

For example, the energy of the first level is $E_1 = -2.178 \times 10^{-18} \text{ J}$, whereas the energy of the third level is $E_3 = -5.44 \times 10^{-19} \text{ J}$; 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 an hydrogen atom. The first level is E_1 and is the most negative energy value, being also the most stable level. In another words, the electrons in this level are tightly bonded to the nucleus. This energy levels is called the fundamental energy level. The following levels (E_2, E_3, \dots, E_n) have a more positive energy. For example, comparing E_2 and E_4 , we have that an electron on the 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 more and more closer to each other. Electrons occupying energy levels with n higher than one are called excited states. Finally, there are infinite number of levels and the highest energy (E_∞) level has an energy of 0J. The electron transitions between the different energy levels is what generates the emission spectrum of hydrogen.

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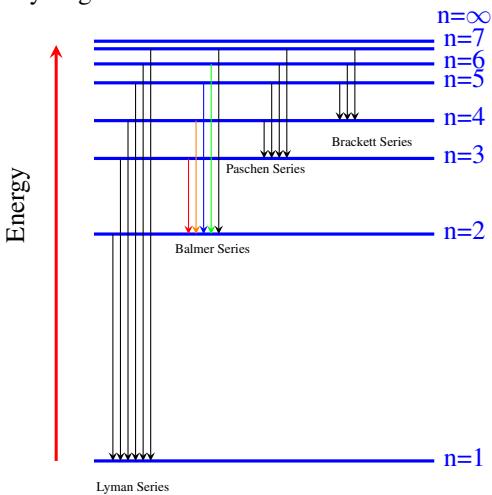


Figure 9.8 Energy levels of Hydrogen and the different emission series. Each series—called Lyman, Balmer, Paschen and Brackett—terminates at a different value of n .

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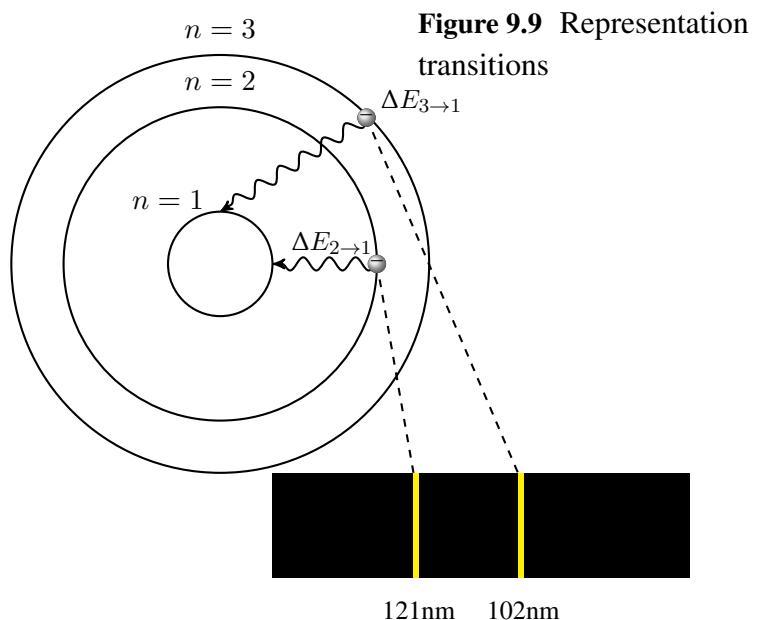
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Transition energies Bohr's models is able to explain the atomic spectrum of hydrogen. Each line in the spectrum represents a transition between two levels of energy. For example the line at 102nm represents the transition of an electron between the level three and the level one, we call this $3 \rightarrow 1$. The atomic spectrum of hydrogen is obtained by means of exciting hydrogen atoms with energy, so that the electron jumps from a lower level into a higher level. When the atom relaxes, it emits light as the electrons move back from high every levels into lower—more stable—levels. This is called an emission. The different possible emissions have names based on the person who discovered them. For example, the set of emissions that end up in the fundamental level ($n=1$) are called the Lyman series. Similarly, the set of emissions that end up in the level ($n=2$) are 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 Bracket series belong to the infrared.

Table 9.3 Emission spectrum of hydrogen

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

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**Figure 9.9** Representation of two energy transitions

Bohr's formula for energy transitions Bohr's formula gives you the values of the energy levels. 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

2460

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:

- (a) $\Delta E_{4 \rightarrow 3}$ in J
- (b) $\Delta E_{4 \rightarrow 3}$ in eV
- (c) 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

- (a) 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.

Answer: (a) $-2.15 \times 10^{-19}\text{J}$; (b) -0.30eV.

The wave properties of matter Bohr's models was able to explain the experimental data for the hydrogen spectrum but still scientist—not even Bohr himself—did not know why electrons were restricted to move in specific orbits.

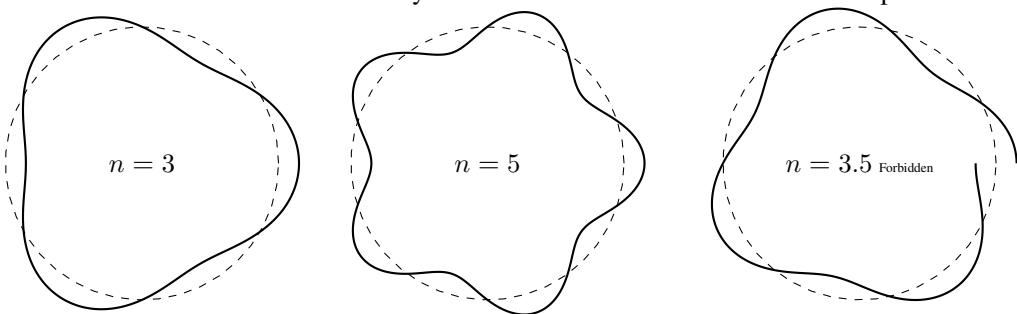


Figure 9.10 In the circular Bohr's orbits, electron could only have wavelengths that are a multiple of the orbit length, or the wave would cancel (forbidden orbits).

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. 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 as the De Broglie wavelength and the mass associated with a wavelength is called 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

$$n\lambda = 2\pi r$$

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:

$$\lambda = \frac{6.6 \times 10^{-34} \text{ Js}}{0.1 \text{ Kg} \cdot 100 \text{ m/s}} = 6.6 \times 10^{-35} \text{ m}$$

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 $9 \times 10^{-31} \text{ kg}$.

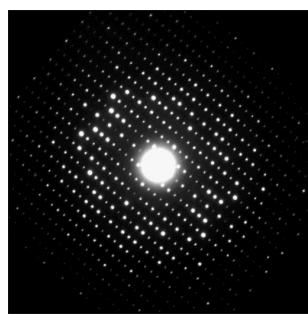
Answer: $7.3 \times 10^{-6} \text{ m}$.

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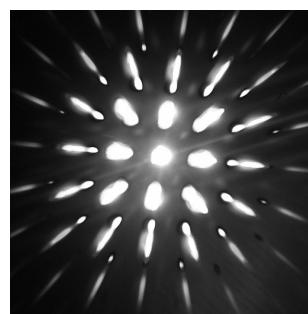
Electron diffraction Following De Broglie's proposal that particles behave like waves under certain circumstances, particles, in particular, electrons were found to exhibit properties of wave. The diffraction of electrons was achieved by Davidsson and Germer by directing a beam of electrons through a thin piece of gold foil creating a pattern similar to the diffraction of x-rays.

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▼Diffraction pattern of electrons ▼Diffraction pattern achieved with a laser



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Figure 9.11 Diffraction patterns produced by light and by matter

9.3 Quantum mechanics and electronic structure

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 describe the structure of the atom: quantum mechanics. The outcome of this section is the existence of orbitals and quantum numbers.

Quantized energy and continuum energy Quantum mechanics is a theory shared in physics and chemistry that describe 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 computer-based modeling to ensure the plane will work properly. In a similar way, chemists carry modeling to describe the properties of chemicals. The theory behind engineering modeling is classical mechanics, based in Newton's law. The theory behind chemistry modeling is quantum mechanics, based in Schrödinger equation. Classical mechanics is based on the idea that the energy of a system, a plane or a car, is 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 in 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 particle through its mass and in terms of wave through a wave-like function, Ψ .

$$\hat{H}\Psi = E\Psi$$

\hat{H} is called hamiltonian operator and contains a 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 simple algebraic equation in which the 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 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. By means of 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 another words is a wave function that contains information of 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 for example a tennis ball. Larger objects are localized, that is they are located at a specific point in space. Differently, electrons are delocalized, that 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 an a specific point. Orbitals are mathematical functions with a radian 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. An 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 movement of the electrons in the hydrogen atom. When we say that an electron is at a given orbital, we mean that the electron density distribution is described by the square of the wavefunction associated with that orbital.

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Orbitals are described by three 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 orbitals Ψ_{n,ℓ,m_ℓ} is characterized by a 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. In the following, we will describe each quantum number separately.

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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.

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l value	Orbital label
0	s
1	p
2	d
3	f

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.

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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 indulging 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.

2540

Quantum number	Values
n	1, 2, 3...
l	0, 1, ..., $n-1$
m_ℓ	$-l, -l+1, \dots, 0, \dots, l-1, l$
m_s	$+1/2$ or $-1/2$

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 $-1/2$.

Sample Problem 89

Indicate if the following combination of quantum numbers is allowed:

n	ℓ	m_ℓ	m_s	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 $\ell = 0$, 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.

n	ℓ	m_ℓ	m_s	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:

n	ℓ	m_ℓ	m_s	Allowed?
4	3	3	$+1/2$	
4	3	3	0	
2	1	-1	$+1/2$	

Answer: yes, no, yes.

2550 *Shells and subshells (or levels and sublevels)* A shell (or a level) is a collection of orbital with the same value of n . 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 .

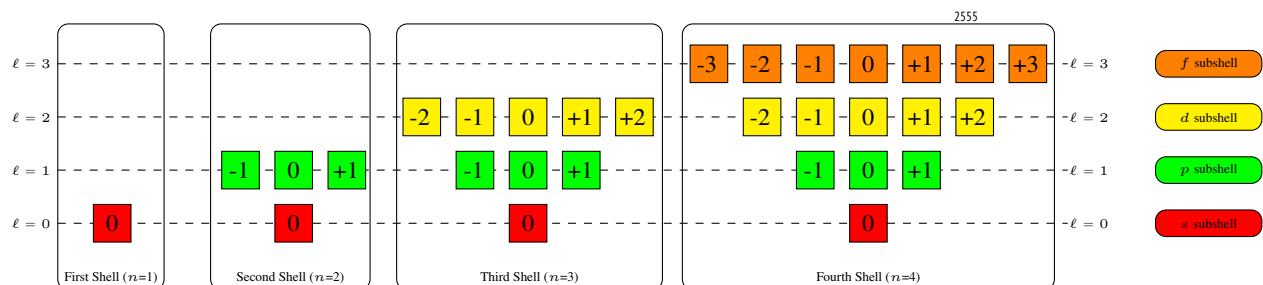


Figure 9.12 The shell and subshell distribution for different principal and angular quantum numbers. Orbitals with the same value of n belong to the same shell and orbitals with the same n and ℓ values belong to the same subshell.

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 $\ell = 0$, whereas p orbitals have $\ell = 1$ and d orbitals have $\ell = 2$. Finally, f orbitals have $\ell = 3$. The principal quantum number should also be indicated before the label. For example, 2560 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.

Different orbitals plots It is not straightforward to represent orbitals, as they extend throughout the space. However, there are three common ways to represent s orbitals, and in general any orbital: (a) by means of the surface that contains 90% of the total electron probability, 2565 (b) by means of the orbital square, and (c) by means of 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.

s orbitals s orbitals are characterized for having $n = 0$. There is a single s subshell 2575 in every shell and each s subshell contains only a single orbital. All s orbitals have an overall spherical shape with increasing size depending on the principal quantum number n . For example, the $1s$ orbital is smaller than the $2s$ and so on. The probability density plot show an interesting feature. For the $2s$ plot, the graph shown a minimum—called a node—representing the distance from the nucleus where the probability of finding an electron is zero. The number of nodes depend on the principal quantum number so that $1s$ orbitals has zero nodes, $2s$ has one node, and $3s$ has two nodes, and so on. The radian distribution plot of 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. 2580 2585

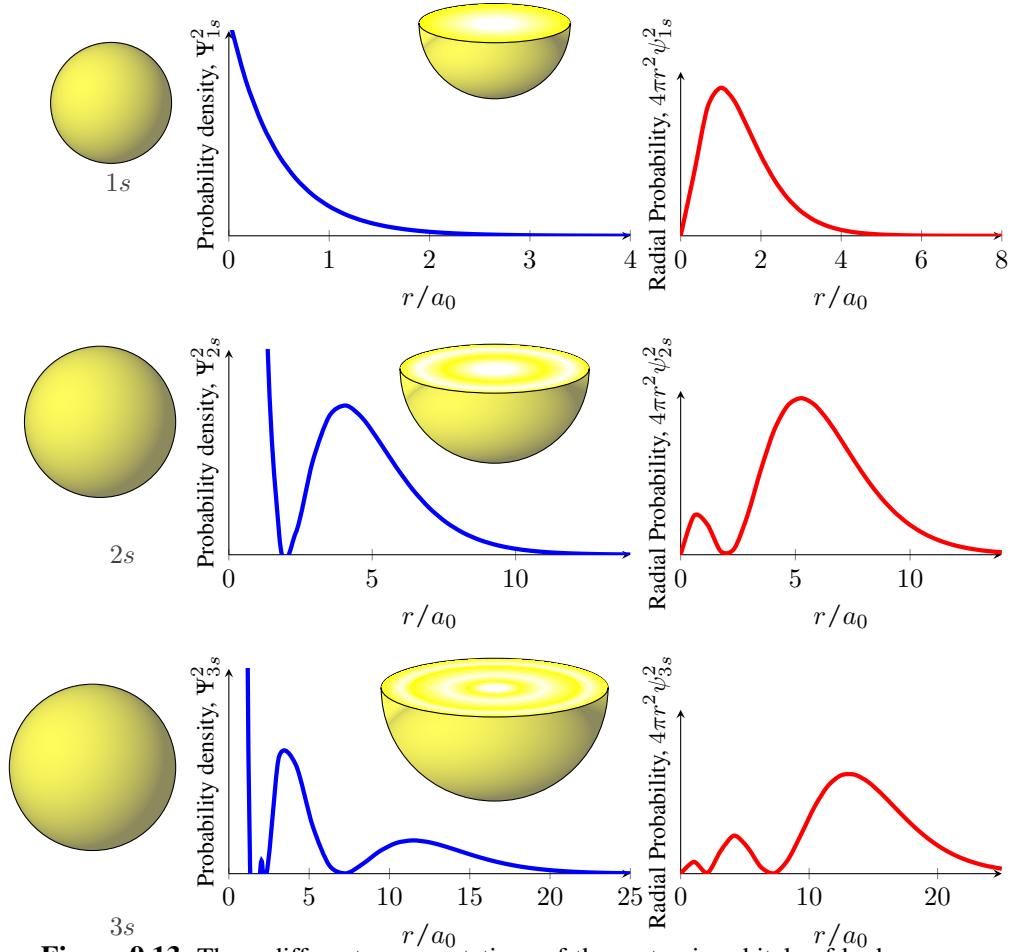


Figure 9.13 Three different representations of the s atomic orbitals of hydrogen: (left) boundary surface plots, (center) probability density plots (the orbital squared) with a sliced 3D surface plots, and (right) radial probability function. The value of a_0 , called Bohn's radius, is 52.9pm. The yellow circles inside the sliced 3D surface plots represent the orbital nodes.

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 $2p_x$. There is no relationship between the subindex labels and the values of m_ℓ . The boundary surface diagrams of p orbitals expose their shape in the form of two lobes, and with positive and one with negative sign.

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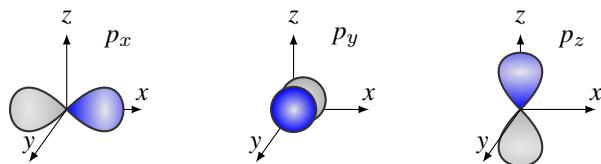


Figure 9.14 Surface plots of the three p orbitals.

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 not related to the quantum number m_ℓ but to the

orientation of the orbital in the 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 not d orbitals in the first or second shell. Regarding the f orbitals, there are seven orbitals with very complex shapes.

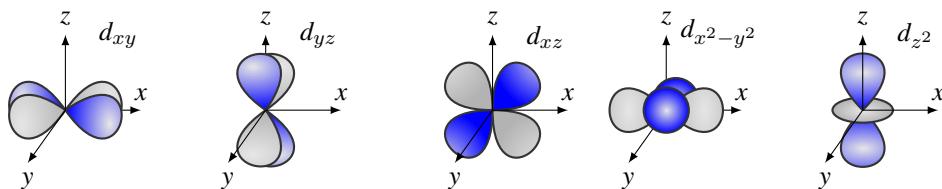


Figure 9.15 Surface plots of the three d orbitals.

Energies of orbitals The orbitals of hydrogen have different energy depending on the principal quantum number. The $1s$ orbital has the most negative–stable–energy. The $2s$ and $2p$ orbitals have both the same energy and overall have a more positive energy than the $1s$. The orbitals at the third shell have a more positive energy than the orbitals in the previous shell. And the trend continues.

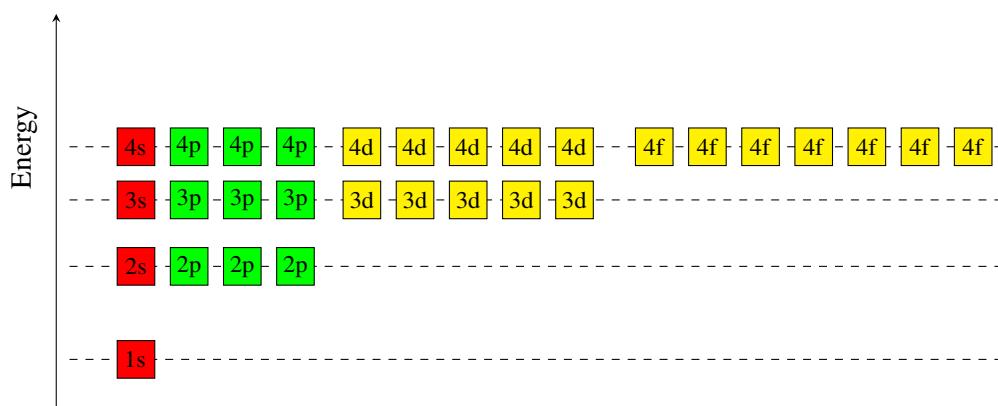


Figure 9.16 Energy of the different hydrogen orbitals. s orbitals have the lowest energy and hence are the most stable. Orbitals in the same shell ($2p$, $2s$) have the same energy. The larger the principal quantum number the more positive the energy, the less stable the orbital.

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The uncertainty principle Waves result from the propagation of energy and are not localized. Electrons behave as waves under certain conditions. In order to approach the problem of trying to locate a particle that behaves as a wave, 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:

$$\Delta x \cdot m \Delta v \geq \frac{h}{4\pi} \quad (9.1)$$

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 $\frac{h}{4\pi}$.

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Sample Problem 90

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.

Answer: $\geq 3 \times 10^3 \text{ m/s}$.

9.4 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 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. In fact, 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 display all orbitals in an atom, whereas the abbreviated only display the valence electrons—these electrons are less-tied to the nucleus—and the noble gas core. At the same time, every orbital is characterized by a set of numbers—these are called quantum numbers. These numbers are not independent from each other and there are constraints that relate the possible values of the quantum numbers. This section will show you how to construct electron configurations and how to extract quantum numbers from it.

Electron energy levels and sublevels The electrons in an atom are arranged in different energy levels. Some levels have lower energy and the electrons 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. Still, each electron in an energy level have the same energy. The energy levels are labeled with a number n that equals to 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 floor 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

$$2n^2 \quad (9.2)$$

in which n is the energy level. You can see by using this formula that for example, the third level can accommodate 27 electrons. Each energy level consists of one or more sublevels, which contain electrons with identical energy. The number of sublevels in each level corresponds to n . For example, in the first energy level ($n = 1$) we have only one sublevel, whereas in the third energy level ($n = 3$) we have three sublevels.

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.

Answer: $n = 9$.

The Pauli exclusion principle The Pauli exclusion principle states that no two electrons in an atom can have the same values of the four quantum numbers. It tells

that each electron is unique and it has to be differentiated with an unique combination of quantum numbers. Because of this, each orbital can only accommodate two different electrons, one with $-1/2$ spin and one with $+1/2$.

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 latest being completely 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 d orbital you can place fourteen or less electrons. For example, the orbital notation p^2 is correct as in p orbitals you can place six or less electrons. In this case, this orbital still have space to accept more electrons. Differently, the notation d^{12} is incorrect, as in d orbitals you can fit ten or less 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 the Figure 9.17. You start from the top of the table and follow the arrows that indicates the orbitals ordering. For examples the first orbital to be filled will be $1s$. After that you should fill $2s$ 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 electrons and $2p^6$ is completely filled. Another example, a $3d$ orbital is empty and can accommodate a maximum of 10 electrons.

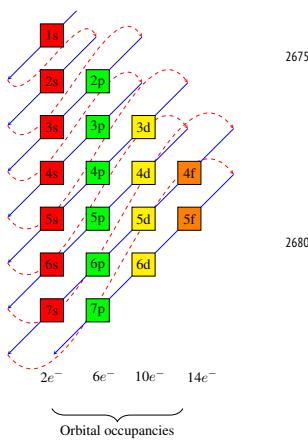


Figure 9.17 Table indicating the orbital filling order. In order to use this table you need to start by filling the orbital $1s$, after that you follow the arrow until next level and start from the beginning of next arrow. For example, after $3d$ you need to fill $6s$. Also the orbital occupancies are given below. s orbitals can fit a maximum of two electrons, whereas p orbitals can fit a maximum of six electrons, as there are three p orbitals (p_x , p_y , and p_z).

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 $1s^2$ and the one for Li is $1s^2 2s^1$. 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 what orbitals to fill? The Figure bellow shows the orbital order. You need to start from the top of the image, from orbital $1s$ and proceed to 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 electronic configuration of C.

SOLUTION

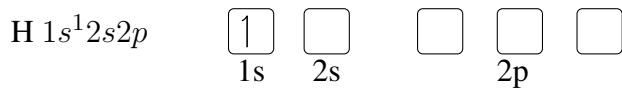
The atomic number of C is $Z=6$ and that means C has 6 electrons. The orbital order from Figure 9.17 is: $1s, 2s, 2p, 3s$, etc. Each s orbital can fit two electrons, whereas the occupancy of the p orbitals is six electrons. Hence the electronic configuration of C is: $1s^2 2s^2 2p^2$. The s orbitals are all filled, whereas the p orbital is only occupied with two electrons.

❖ STUDY CHECK

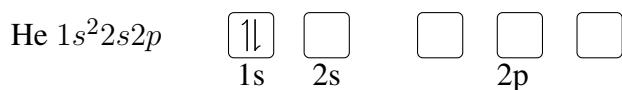
Obtain the electronic configuration of Ni.

Answer: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$.

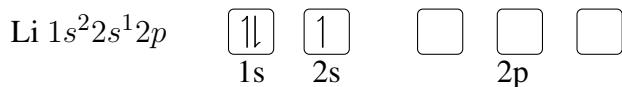
2700 *Hund's rule* Let us build up the electron configuration of a series of atoms. Starting with hydrogen, with one electron, we have that only the $1s$ orbitals will be filled:



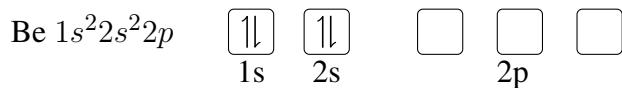
For the case of helium, with two electrons, we have that based on Pauli's principle both electron have different quantum numbers and in order to differentiate this we will represent the pair of electron with arrows in opposite direction. We say both electrons are paired:



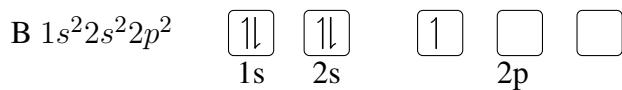
Now, for the case of Lithium and Beryllium we have a similar situation. Lithium has a single unpaired electron and Beryllium has a set of paired electrons in the $2s$ orbital:



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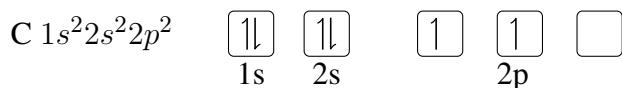


The next element, Boron, has one electron in a p orbital. As all p orbitals are degenerate—they have the same energy—we can place that single electron in any of the p orbitals. Normally, we use the one on the left:

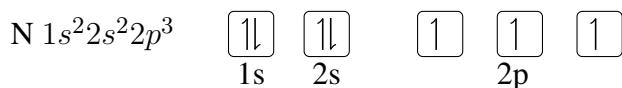


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For the case of Carbon, as we need to place two electrons in the p orbitals, Hund's rule states that we need to place the electron maximizing the number of unpaired electrons. In another words, the second electron goes into a separate p orbital, just like below:

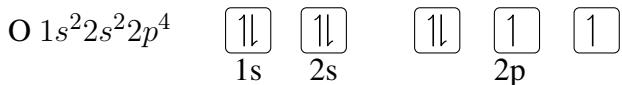


Similarly, for the case of Nitrogen we have:

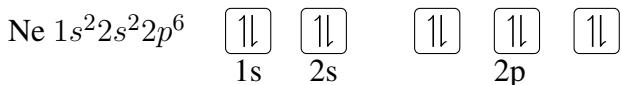


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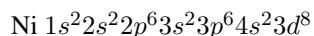
Now, for the case of oxygen, as we cannot place that extra electron in a separate p orbital we have to start pairing electrons:



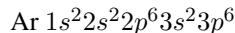
Finally, for the case of Neon we have the whole second shell filled with electrons:



Abbreviated Electron Configuration and orbital diagrams Let us compare the electronic configuration of Ni and Ar. We have:

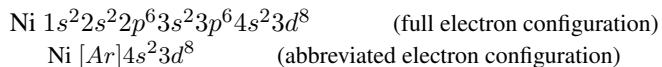


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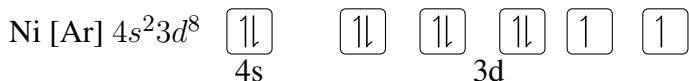


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We called these configuration the *full electronic configuration*. If you look carefully, you will see that both configurations resemble and in particular the configuration of Ni is the same as the configuration of Ar with two extra orbitals added. 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:



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We call this last configuration as 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 the 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 [Ar] with 18 electrons, and the remaining 10 electrons (Ni has 28 electrons) starting by the orbital 4s, according to the 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, it has 18 core electrons in the Ar core and 10 electrons in the valence. Let us work another example: Cd. It has 48 electrons, and is located in group 5. The noble gas on 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 belong to period five. In the valence electrons, we will place 12 electrons. Hence, the abbreviated configuration will be: $[\text{Kr}] 5s^2 4d^{10}$.

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Sample Problem 93

Obtain the full and abbreviated electronic configuration of Silver (Ag, Z=47).

SOLUTION

The atomic number of Ag is Z=47 and that means Ag has 47 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. d orbitals can fit 10 electrons. 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: $[Kr]4d^{10}5s^1$. Ag has 36 core electrons and 11 valence electrons.

 **STUDY CHECK**

Obtain the abbreviated electronic configuration of Cobalt (Co, Z=27).

Answer: $[Ar]3d^7 4s^2$.

9.5 Periodic Trends

Some atomic properties are periodic, which means that they follow a certain trends in the periodic table. These properties increases or decreases across a period and then the trend is repeated again in each successive period or group. We will consider here four atomic properties: the atomic size, the ionization energy, the metallic character and the electronegativity.

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 the nuclear charge creating an effective nuclear charge. This way, the effective nuclear charge is the actual magnitude of positive charged experienced by an electron. In many-electron atoms, an electron is partially shielded from the positive charge of the nucleus. Among the different types of electrons in an atoms (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.

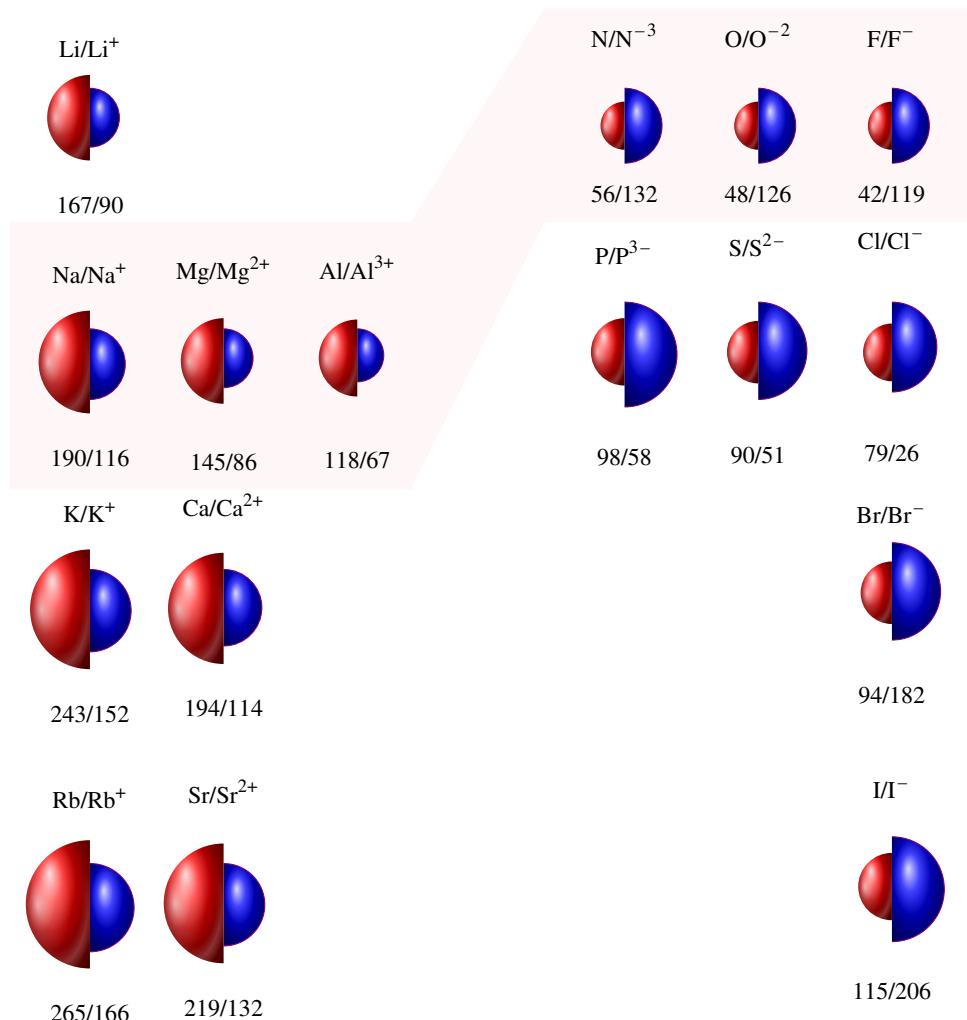


Figure 9.18 Ionic and atomic radius across the periodic table

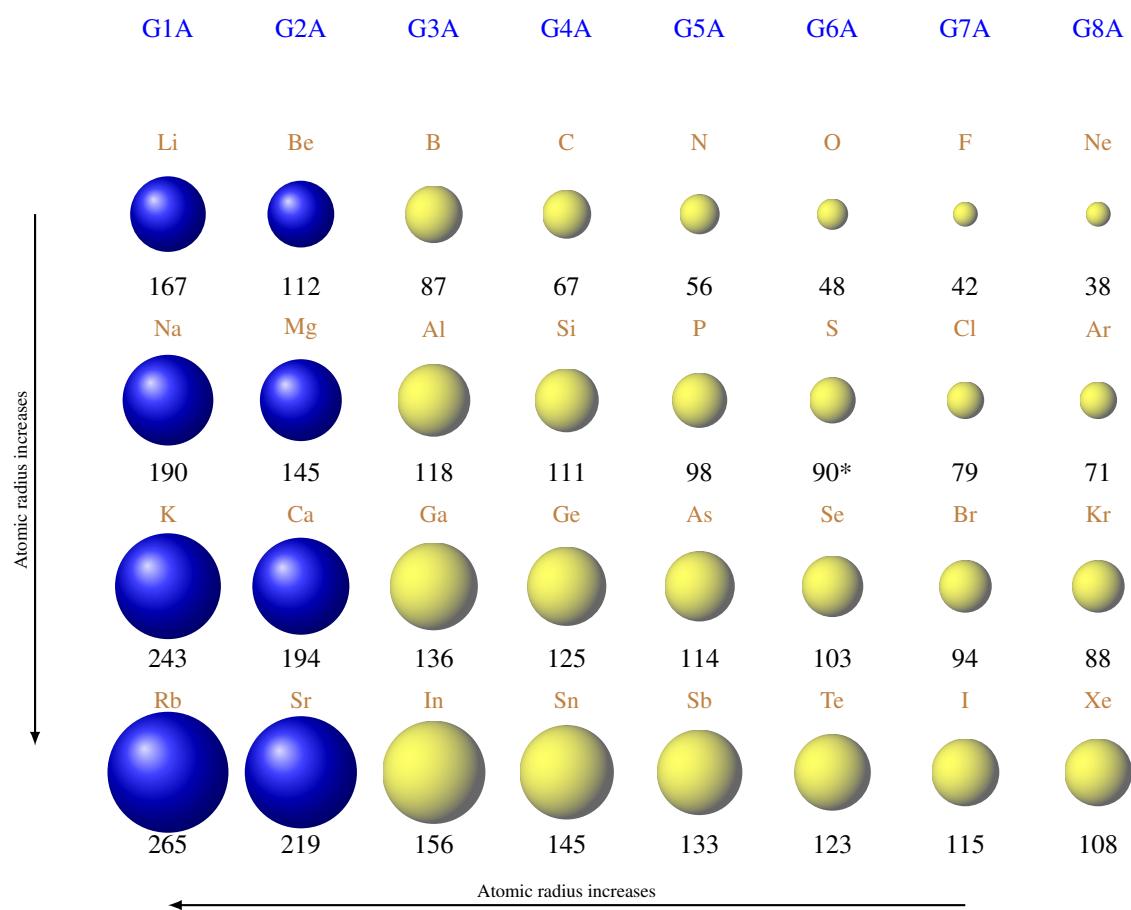


Figure 9.19 Change of atomic radius (calculated values given in pm) across the periodic table. The value with * was estimated

2765 *Ionization Energy* The *ionization energy* (IE) is the energy needed to remove an electron from an atom in gas state and its fundamental (ground) electronic state. Atoms can have numerous ionization energies. 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.

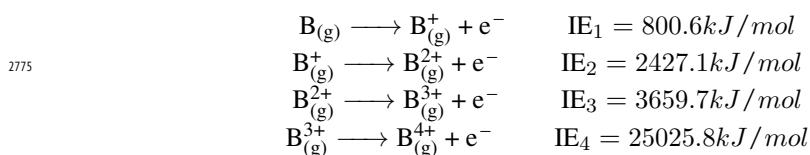
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Table 9.4 Ionization energy in the periodic table in kJ/mol

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

For the case of boron,



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Given the electron configuration of Boron ($[\text{He}]2\text{s}^22\text{p}^1$), 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.

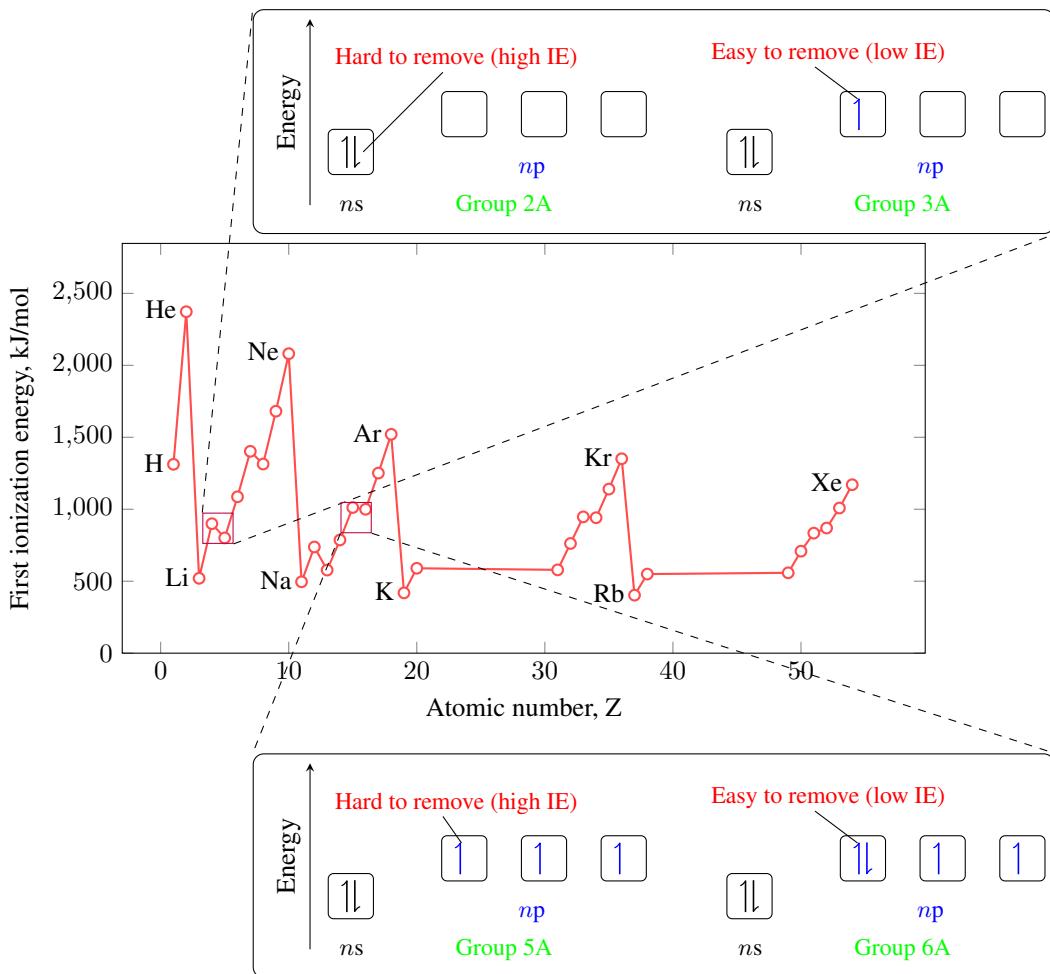


Figure 9.20 Ionization energy graphed with respect to the atomic number

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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 the metals and high for the 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 ($\text{IE}_H < \text{IE}_{He}$). For the case of Li and H, the EI will be higher for H as it is further up in the same group ($\text{IE}_H > \text{IE}_{Li}$). There are discontinuities in the IE when moving across a period. Table 9.4 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

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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.

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:



2800

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 electron 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.

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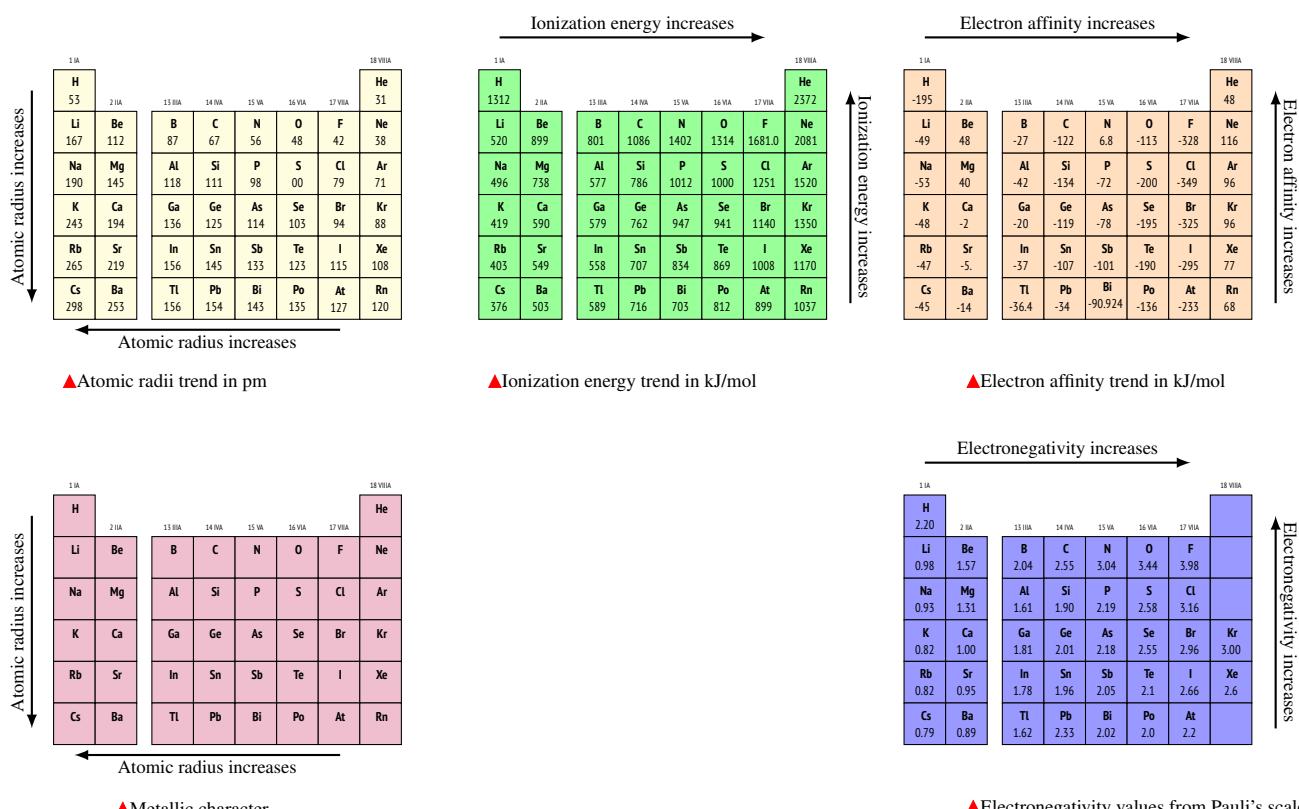


Figure 9.22 Periodic properties across the periodic table

Electronegativity, EN Atoms combine with each other by sharing or give 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 person is more electronegative it will pull the pillow closer to them—it will attract more the electrons. Electronegativity is loosely related to other periodic properties such as ionization energy and the 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) increase (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 in relation to 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 ($EN_F > EN_I$).

2835 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 in 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 ($MC_K > MC_{Ca}$). For the case of F and Cl, Cl is more metallic as it is located further down a group ($MC_{Cl} > MC_F$).

Sample Problem 94

Compare the following property for the given couple of elements:

- Atomic radius of N and F.
- Ionization energy of Na and Cs.
- Electronegativity of F and I.
- 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.

Answer: (a) radius I > F; (b) Electronegativity Na > Cs.

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 common electronic configurations. For example, Na^+ and F^- both have the electron configuration: $[\text{He}]2s^22p^6$. 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. The figure below, shows the changes of ionic radii across the periodic table.

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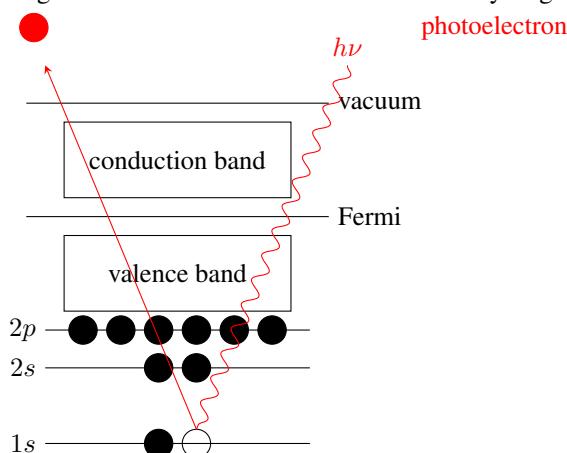
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Photoelectron spectroscopy of atoms Photoelectron spectroscopy is a technique used to measure the relative binding of the electrons of an atom. It is useful to experimentally obtain the energy levels of an atom and properties such as the ionization energy. The principle behind the technique is similar to the photoelectric effect. By shining light with enough energy one can remove electrons of an atom. 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 lights, 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 present a series of characteristic peaks. However, there are many factors that affect the photoelectron picks and for example an 1s peak of H can appear at different energies depending on the nature of the atom bonded to hydrogen.

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Figure 9.23 A photo-electron emitted from a 1s level



In general, in 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 for 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.

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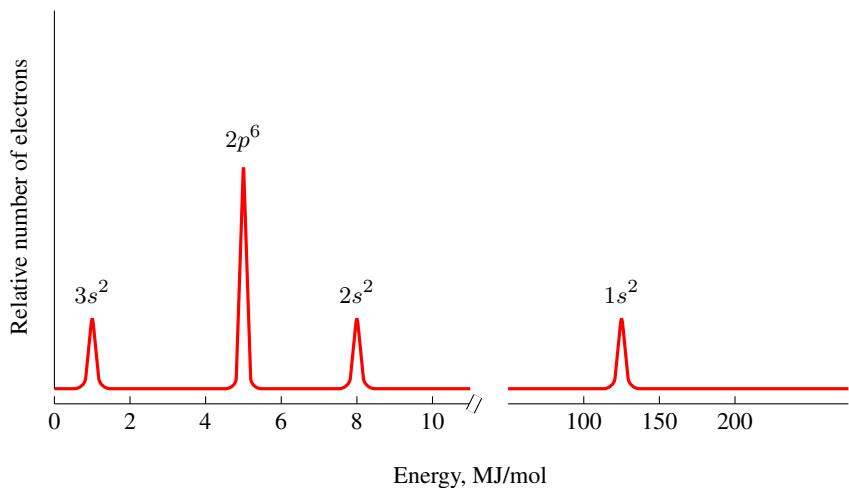


Figure 9.24 Photoelectron spectrum (PES) of Magnesium

CHAPTER 9

THE NATURE OF LIGHT

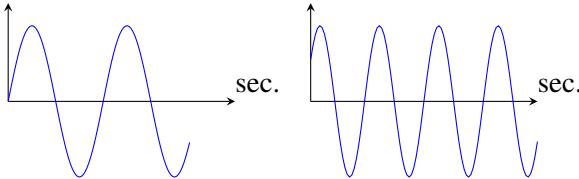
9.1 Calculate the following properties: (a) The energy in joules of a radiation with frequency 2.0×10^{18} Hz? (b) The frequency of a radiation with energy 5.6×10^{-20} J? (c) The energy in joules of a radiation with wavelength 653 nm?

9.2 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?

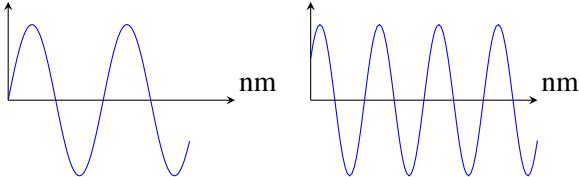
9.3 Calculate the following properties: (a) The color of a radiation with $\lambda = 510$ nm. (b) Indicate the color of a radiation with $\lambda = 580$ nm.

9.4 Classify the nature of a radiation (a) A radiation with $\gamma = 3.4 \times 10^8$ Hz (b) A radiation with $\lambda = 1 \times 10^{-4}$ nm

9.5 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?



9.6 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

9.7 Which of these electron transitions correspond to absorption of energy and which to emission?

- | | |
|----------------------------------|----------------------------------|
| (a) $\Delta E_{1 \rightarrow 2}$ | (d) $\Delta E_{3 \rightarrow 5}$ |
| (b) $\Delta E_{2 \rightarrow 1}$ | (e) $\Delta E_{5 \rightarrow 3}$ |
| (c) $\Delta E_{3 \rightarrow 1}$ | (f) $\Delta E_{1 \rightarrow 3}$ |

9.8 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 $n = 4$.

9.9 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 $n = 5$.

9.10 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 AND ELECTRONIC STRUCTURE

9.11 Indicate the number of orbitals that can have the following designations: (a) 2s (b) 3p (c) 0p (d) $n = 4$

9.12 Indicate if the following combination of quantum numbers are allowed:

n	ℓ	m_ℓ	m_s	Allowed?
4	4	1	$+1/2$	
2	1	4	$+1/2$	
4	2	-2	$-1/2$	

9.13 For each of the following sublevels, give the n and ℓ values and the number of orbitals: (a) 6s (b) 4d (c) 2p

9.14 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) $[Kr]5s^2 4d^8$

PERIODIC PROPERTIES

9.15 Among the elements, indicate the element with the largest atomic radius (a) B (b) C (c) F (d) Li (e) Na

9.16 Among the elements, indicate the element with the largest ionization energy (a) B (b) C (c) F (d) Li (e) Na

9.17 Among the elements, indicate the element with the largest electronegativity (a) B (b) C (c) F (d) Li

9.18 Among the elements, indicate the element with the largest metallic character (a) B (b) C (c) F (d) Li (e) Na

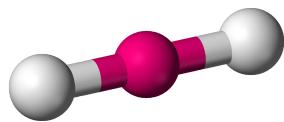
Answers **9.1** (a) $1.32 \times 10^{-15}\text{J}$ (b) $8.5 \times 10^{13}\text{Hz}$ (c) $3.03 \times 10^{-19}\text{J}$ **9.3** (a) Green (b) Yellow **9.5** (a) $\gamma_A < \gamma_B$ (b) $E_A < E_B$ (c) IR **9.7** (a) Absorption (b) Emission (c) Emission (d) Absorption (e) Emission (f) Absorption **9.9** $3.16 \times 10^{15} \text{ Hz}$ **9.11** (a) 1 orbital (b) 3 orbitals (c) 0 orbital (d) 16 orbitals **9.13** (a) 6s ($n = 6; \ell = 0$) (b) 4d ($n = 4; \ell = 2$) (c) 2p ($n = 2; \ell = 1$) **9.15** Na **9.17** F

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Electronic structure of molecules

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In nature molecules can be found in a myriad of different shapes. Some like carbon dioxide are one-dimensional or linear, others like methane have a shape that expands in the three directions of the 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 to 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.



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GOALS

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- 1 Construct electron-dot structures
- 2 Identify the geometry of a molecule
- 3 Identify the polar character of a molecule
- 4 Calculate the bond hybridization
- 5 Interpret molecular orbital diagrams

Discussion: oil spills on your shirt during a dinner. List three chemicals than can remove the stain

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10.1 Electron-dot structures of atoms

Atoms are made of protons, neutrons, and electrons. Electrons—in particular valence electrons—are responsible for the main chemical properties of an atom. These electrons are tied weakly to the nucleus in comparison with the core electrons and hence they can be exchanged easily with other atoms. Atoms in a molecule, with a few exceptions such as the hydrogen case, will tend to be surrounded by eight electrons so that its electron configuration resembles a noble gas. This is known as the octet rule (the duet rule in the case of hydrogen), and 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^+ ($[He]2s^22p^6 = [Ne]$). The electron-dot structure of an atom or a molecule is a visual representation of the electronic arrangement in an atom or a molecule.

Valence electrons The electrons of an atom can be divided in 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 in an atom is the same as the group number. As an example, hydrogen H belongs to the group IA and hence has one valence electrons. Similarly, oxygen O belongs to the group VIA and therefore it has six valence electrons.

Sample Problem 95

Indicate the number of valence electrons for the following atoms: N, O, C and S.

SOLUTION

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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

 **STUDY CHECK**

Indicate the number of valence electrons for the following atoms: Cl and B.

Answer: Cl ($7e^-$), B ($3e^-$).

The octet rule Atoms gain or lose 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 claims that each atom in a molecule is normally surrounded by eight (octet) electrons. There are two important exceptions to this rule as H is only surrounded by two electrons (this is called the duet rule), and B by six.

Electron-dot structure of an atom In order to write the electron-dot structure of an atom, you just need to write down the symbol of the atom surrounded by the number of valence electrons one by one four directions, and if you have more than four electrons then add remaining electrons as pairs. For example, oxygen has six valence electrons and hence, the electron-dot structure would be $\cdot\ddot{\text{O}}:$ Similarly, for the case of fluorine the the electron-dot structure would be $\cdot\ddot{\text{F}}:$ In the case of an ion, you need to add (if its an anion) or subtract (if its a cation) electrons, and for example the electron-dot structure of O^{2-} is $\cdot\ddot{\text{O}}:^{2-}$

Sample Problem 96

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 $\cdot\dot{\text{C}}\cdot$. Cl^- has eight valence electrons, that is seven plus one, and hence its electron-dot structure will be $\cdot\ddot{\text{Cl}}:^-$.

 **STUDY CHECK**

Write down the electron-dot structure for N^{3-}

Answer: $\cdot\ddot{\text{N}}:^{3-}$.

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Electron-dot structure of diatomic molecules This section will address how to build up electron-dot structures of diatomic molecules. These would be the most simple electron-dot structures of molecules that you will see. The first step is (a) to set up the atoms in the molecule in the form of a line. After that, (b) 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, O is 6 as its group is VIA). Then you (c) compute the pairs of electrons—the total number of valence electrons divided by two; pairs of electrons are represented by lines. In the following (d) you need to start distributing the pairs in the molecule in a very specific way: first connecting the atoms among themselves, and after placing the remaining pairs surrounding the atoms. Overall, each atom should be surrounded by four pairs with the exception of H and B.

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Sample Problem 97

Construct the electron-dot structure of HCl.

SOLUTION

- 1 **Step one:** we first arrange the atoms in the molecule as H Cl.
- 2 **Step two:** now we count the number of valence electrons: H(1) and Cl(7) 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. H: $\ddot{\text{C}}\text{l}$:; using lines instead of pairs (this is not necessary but makes the electron-dot structure look better) we obtain H— $\overline{\text{Cl}}$.

◆ STUDY CHECK

Construct the electron-dot structure of HF.

Answer: H— $\overline{\text{F}}$.

Electron-dot structure of general molecules Now we will address how to build up electron-dot structures of more complex molecules. The first step is (a) 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, (b) you need to count the total number of valence electrons in the molecule, by adding the valence electrons of each atoms. Then you (c) calculate the pairs of electrons—the total number of valence electrons divided by two; pairs of electrons are represented by lines. In the following (d) you need to start distributing the pairs in the molecule in a very specific way (this is the key to building good electron-dot structures): first connecting the surrounding atoms to the central atom, after placing pairs on top of the surrounding atoms and finally by placing the remaining pairs in the central atom. Each atom should be surrounded by four pairs (this is the octet rule) with the exception of H and B as they do not follow the octet rule. When you have the final electron-dot structure, the pairs of electrons (or lines) that connect two atoms are called *bonds*, whereas the pairs not involved in an connection are called *lone pairs*. A very important note is that, at this point, is not that 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 in the surroundings) is correct.

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Sample Problem 98

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: $2 \times H(1)$ and 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. $H:\ddot{O}:H:$ and using lines instead of pairs (this is not necessary but makes the electron-dot structure look better) we obtain $H-\overline{O}-H$. 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..

Answer: $H-\overline{N}-H$; three bonds and one lone pair.

|
H

Atomic charges in a molecule In order to build up the electron-dot structures of a molecule you need to count the number of valence electrons. Each atom brings a different number of valence electrons to a molecule. For example, H brings one whereas O brings two. When you arrange the electron pairs in the molecule, each atom should have the number of electrons that they bring. For example in this electron-dot structure $H:\ddot{Cl}:$ the hydrogen atom brings one electrons to the molecule, and in the molecule the atom owns one electrons, as in $H:$ one of the dots belong to H and the other belongs to the Cl—the electrons are shared in a covalent bond. In the same way, the Cl atom brings seven electrons and in the molecule it owns seven electrons, and has six electrons here $\ddot{Cl}:$ plus the one that shared with the hydrogen atom. In another words, the $H:\ddot{Cl}:$ electron-dot structure is the combination of $H\cdot$ and $\cdot\ddot{Cl}:$. We say that the charges on each atom are zero, as each atom in the molecule owns the same number of electrons that it originally brings.

Sample Problem 99

Indicate the atomic charges on each of the atoms of $H-\overline{C}-H$

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).

STUDY CHECK

Indicate the atomic charges on each of the atoms of $H-\overline{N}-H$

Answer: H(0) and N(-1). $H-\overline{N}\ominus-H$

Multiple bonds Often times you are going to encounter electron-dot structures like $\text{:N}\equiv\text{N:}$ in which the atoms are connected by means of a triple bond. You will also encounter double bonds :O=O: and single bonds. These are called multiple bonds and are formed while constructing electron-dot structures in order to avoid having atoms with atomic charges different than zero. Charged atoms in a molecule are in general not favorable. When you build electron-dot structures and you end up having large atomic charges, you can avoid that by moving electrons from the atom into the bond, hence creating multiple bonds.

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Sample Problem 100

Construct the electron-dot structure of O_2 .

SOLUTION

- 1 **Step one:** we first arrange the atoms in the molecule as O O .
- 2 **Step two:** now we count the total number of valence electrons, including all atoms: $2 \times \text{O}(6)$ that gives a total of twelve electrons.
- 3 **Step three:** let us count the pairs of electrons; we have twelve electrons and that is six pairs.
- 4 **Step four:** now we distribute the pairs, first connecting the atoms $\text{O} - \text{O}$ (we have five extra pairs to distribute at this point).
- 5 **Step five:** we place the remaining pairs on top of the oxygen atoms $\langle \overline{\text{O}} - \text{O} \rangle$
- 6 **Step six:** now we calculate the charge on each atom $\langle \overline{\text{O}}^- \oplus \text{O}^+ \rangle$
- 7 **Step seven:** in order to eliminate the charges we move lone pairs into the bond $\langle \text{O}=\text{O} \rangle$. Now the charges are zero and this is more important than imposing the octet rule.

◆ STUDY CHECK

Construct the electron-dot structure of CO_2 .

Answer: $\langle \text{O}=\text{C}=\text{O} \rangle$

10.2 Molecular shape

Molecules are arrangements of atoms, and these arrangements can be presented in different form. Let us use as an example the H_2O molecule, which contains two hydrogen atoms and one oxygen. Knowing that both hydrogens are connected to oxygen by means of a covalent bond, one can envision several molecular geometries such as $\text{H}-\overline{\text{O}}-\text{H}$ or maybe $\text{H}-\overset{\text{O}}{\text{H}}$. The goal of this section is to identify the geometry of a given molecule. In order to do this, the electron-dot structure of the molecule are the key.

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ABE Molecular code If the molecule contains two atoms, there is only a possible geometry these two atoms can exhibit, and this is a linear arrangement. For the case of more complex molecules, in order to identify the geometry you need to figure out the ABE code of the molecule. In this code B refers to the number of atoms connected

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to the central atom in a molecule, and E is the number of lone pairs on the central atom. For example, the electron-dot $\text{H}-\overline{\text{O}}-\text{H}$ structure has two bonds with the central atom B₂ and two lone pairs on top of the central atom E₂ and hence the ABE code of the molecule would be AB₂E₂. Another example the ABE code for ammonia H— $\begin{array}{c} \text{N} \\ | \\ \text{H} \end{array}$ —H would be AB₃E, as the molecule has three atoms connected to the central nitrogen and N has a single lone pair. You can find a list of the equivalence between ABE codes and the molecular geometry in Table ??.

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In order to predict the geometry of a molecule, once you have the ABE code, Table ?? will give you the geometry. For example, an AB₂ molecule will be linear, whereas an AB₂E₂ is bent. The bond angles are also indicated in the table, and for example a CO₂ molecule, which will be linear will have a 180° angle. This means both C-O bonds will form a line.

Table 10.1 Molecular geometries

ABE Code	Molecular shape	Bond Angle	3D model	ABE Code	Molecular shape	Bond Angle	3D model
AB ₂	Linear	180°		AB ₄ E	see-saw	180°, 120°, 90°	
AB ₃	Trigonal Planar	120°		AB ₃ E ₂	T-shaped	90°, 180°	
AB ₂ E	Bent	120°		AB ₂ E ₃	Linear	180°	
AB ₄	Tetrahedral	109°		AB ₅ E	square pyramidal	90°	
AB ₃ E	Trigonal pyramidal	109°		AB ₄ E ₂	square planar	90°, 180°	
AB ₂ E ₂	Bent	109°					
AB ₅	trigonal bipyramidal	90°, 120°, 180°					
AB ₆	octahedral	90°, 180°, 180°					

Sample Problem 101

Identify the geometry of the following molecules: BF₃ and SO₂.

SOLUTION

We need first the electron-dot structure of both molecules. For BF₃ $\begin{array}{c} |\overline{\text{F}}| \\ | \quad | \\ \text{B} - \overline{\text{F}} \end{array}$. The code of this molecule is AB₃ and hence its geometry would be trigonal planar. The correct way to draw the molecule respecting its geometry would be: $\begin{array}{c} |\overline{\text{F}}| \\ | \quad | \\ \text{B} - \overline{\text{F}} \end{array}$. The electron-dot structure for sulfur dioxide—remember this is covalent molecule—is $\begin{array}{c} |\overline{\text{O}}| = \overline{\text{S}} = |\overline{\text{O}}|$ and its class is AB₂E. Hence the molecular geometry is linear.

◆ STUDY CHECK

Identify and draw the geometry of methane (CH₄).



10.3 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 the bond. Polar bonds results in the existence of a permanent dipole moment that makes a molecule polar. Polar molecules can interact with polar molecules and mix.

Bond polarity Let us compare two different molecules: H₂ and HCl. We say H₂ is a non-polar molecule. The reason for this is that each atom in the covalent H-H bond equally share the electrons. Differently, HCl is a polar molecule, as H is an electropositive atom and Cl is electronegative. That implies that in the H-Cl covalent bond each atoms shares the electrons in the bond differently. H will be less prone to attract the electrons and Cl would tend to attract the bond electrons more than H. The result would be that the electrons in the bond would belong more to Cl than to H. Another consequence is that the molecule would have a permanent dipole—a permanent charge distribution—result of a uneven charge distribution in the chemical bond. We represent excess of charge as on Cl as Cl^{δ-} and electron deficiency in H as H^{δ+}. The polarity of the bond is represented as:



Polarity of diatomic molecules Molecules can either be polar or non-polar.

The polarity of diatomic molecules only depends on the nature of the atoms that forms the molecule. If the atoms in the molecule are the same (e.g. H₂ or O₂), then the molecule would be non-polar. If the atoms are different then the molecule would be polar. Examples are H₂ a nonpolar molecule and HCl or HBr, both polar molecules. You can apply the same concept to a bond inside a molecule. The C-O bond in a CO₂ molecule is a polar covalent bond, as C and O have different electronegativities.

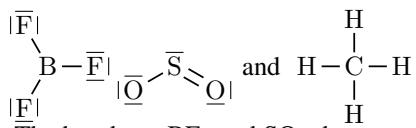
Polarity of larger molecules The polarity of larger molecules would depend on the molecular geometry. Let us analyze the case of CO₂. Each of the C-O bonds on the molecule are polar bonds. However, CO₂ is a linear molecule $\text{O}=\text{C}=\text{O}$ and the polarity of each C-O bonds compensate so that at the end the molecule is polar. For the H₂O case, again, the H-O bond is polar. However, the molecule is bent and looks just like $\text{H}-\overset{\text{O}}{\text{O}}-\text{H}$. Both H-O bonds do not compensate as they point in different direction and the directions do not cancel out what makes the water molecule to be a polar molecule.

Sample Problem 102

Identify the polar character (polar/nonpolar) of the following molecules: BF₃, SO₂ and CH₄.

SOLUTION

Let us analyze the geometries of the three molecules:



The bonds on BF_3 and SO_2 do not cancel out, as they do not point in opposite directions. Hence these two molecules are polar. On the other hand, the bonds on methane cancel each other out and hence even when the C-H bond is polar, the molecule would be non-polar.

STUDY CHECK

Identify the polar character (polar/nonpolar) of the following molecules: O_2 and NH_3 .

Answer: O_2 is non-polar and NH_3 is polar.

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Polarity and mixing When you mix two different liquids or even gases, polarity is the key for the mixing process. If the molecules have the same polar character they will be able to mix, whereas they will not mix when the polar character is different. This section will cover several examples of mixing an polarity.

3045 *Molecules with the same polarity* Water (H_2O) is a polar molecule. The ABE type of water of AB_2E_2 and hence its geometry is bent. That means both H-O bonds, which are polar, do not compensate with each other. Hence, the molecule will have a dipole moment and hence will be polar. Methanol (CH_3OH) is a polar molecule as well. The central atom of the molecule (C) is connected to three hydrogens and a 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. 3050 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 3055 with the same polarity (polar-polar or nonpolar-nonpolar) will mix.

3060 *Molecules with the same polarity* CCl_4 is a nonpolar molecule, and H_2O is a polar molecule. As both have different polar character they will not mix together. If you mix water and CCl_4 , tow 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 together. Soap has a polar and non-polar part. In order to remove oil from water, soap helps mixing both polar water and nonpolar oil.

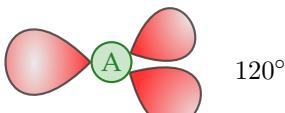
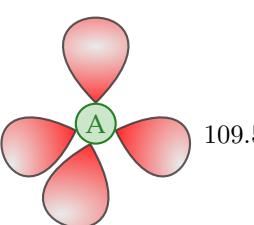
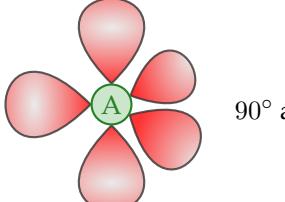
10.4 Hybrid orbitals

3065 Lewis structures are just representations of the bonds in a molecule. These representations are based on the localized electron bonding model, that assumes that molecules are made of atoms that share pairs of electrons. This section will addressed more advanced models. In particular hybrid orbitals are mixtures of atomic orbitals in a molecule. Atoms contains electrons and these electrons are located in atomic orbitals. We call these atomic orbitals 3070 as they belong to atoms. When a few atomic orbitals mix together, they hybridize, that

is they mingle forming combinations of orbitals called hybrid. For example, when a *s* orbital hybridizes with a single *p* orbital, we obtain a hybrid *sp* orbital. At the same time, the *s* orbital can hybridize with two different *p* orbitals forming a *sp*² hybrid orbital. Hybrid orbitals are just a continuation of lewis structures and one can only obtain the hybrid orbitals of an atom in a molecule by means of the lewis structure. Therefore, at this point is very important you master the construction of lewis structures.

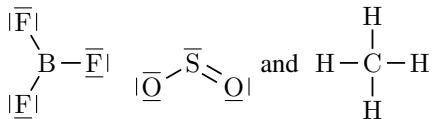
From ABE code to hybridization In order to obtain the hybridization of an atomic center in a molecule we just need the ABE code and Table ???. For example, if the code of a molecule is AB₄, the hybridization of the molecule will be *sp*³. Similarly, if the class is AB₃ the hybridization will be *sp*² 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 AB₄E. This time, the hybridization would be *sp*³*d*². Mind that in general the number of hybrid orbitals correspond to adding the E and B from the class. For example, AB₄E₂, 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.

Table 10.2 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 <i>d</i>		90° and 120°

Sample Problem 103

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 .

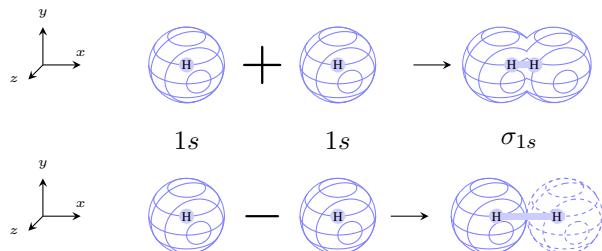
Answer: sp and sp^3 .

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10.5 Molecular orbital theory

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 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, result from the constructive combination, and another one called antibonding orbital, resulting from the destructive combination. In this section we will learn how to interpret molecular orbital diagrams.

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 a higher more 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 $1s$ orbital 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.



Sigma and pi orbitals Let's analyze now the mixing of two $2p_x$ orbitals of two oxygen atoms in order to make an O_2 molecule. Mind that p orbitals look like dumbbells and each side of the dumbbell is called lobe. In the p_x orbital the positive lobe is in 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. Differently, if we combine two $2p_y$ orbitals we will obtain two π orbitals, as the lobes of the molecular orbital is perpendicular the axes of the molecule being formed

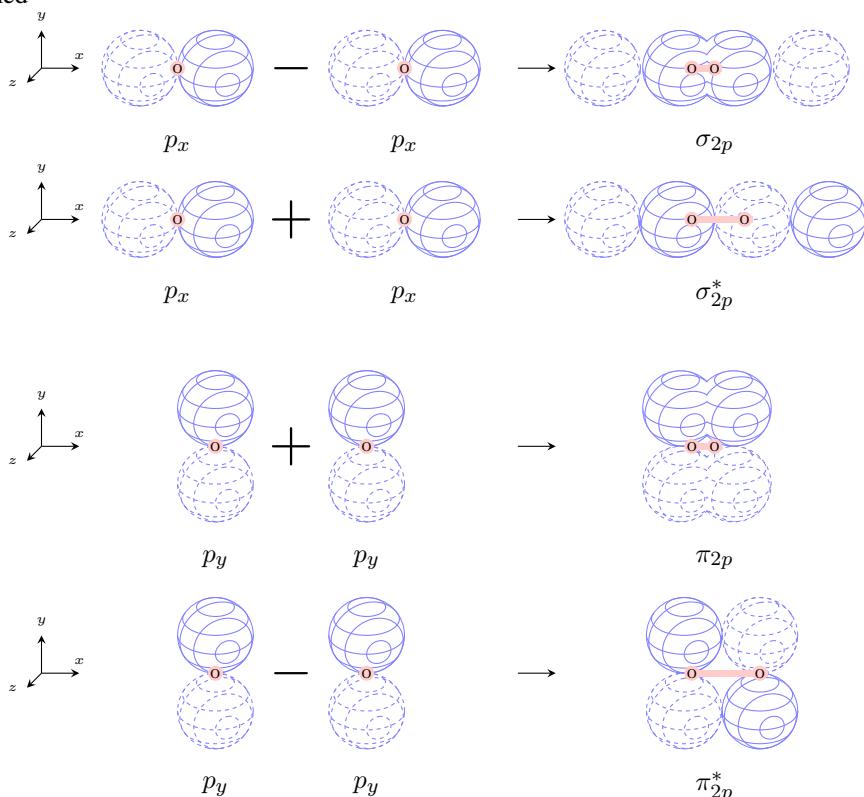


Figure 10.2 (Top) Bonding and antibonding σ orbitals resulting of combining two $2p_x$ atomic orbitals of Oxygen. (Bottom) Bonding and antibonding π orbitals resulting of combining two $2p$ atomic orbitals of Oxygen.

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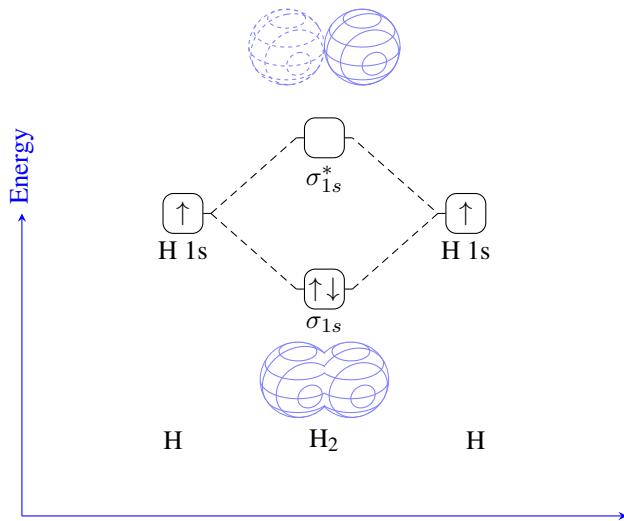
The first orbital is bonding as both lobes overlap constructively, whereas the second orbital is antibonding as both lobes cancel out.

The case of H_2 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

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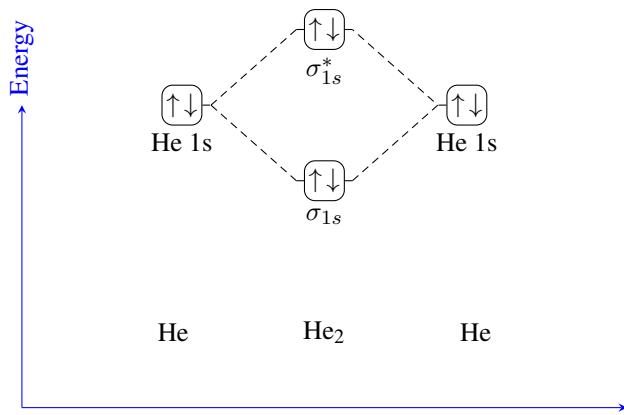
the reason why the hydrogen molecule is a stable existing molecule and takes energy to break down this molecule into atoms.



The case of He₂ molecule Let us analyze the case of the formation of the hypothetical Ne₂ 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: $\text{He}_2 = \sigma_{1s}^2 \sigma_{1s}^{*2}$. 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 He₂ molecule will not be stable in compared to the atoms:

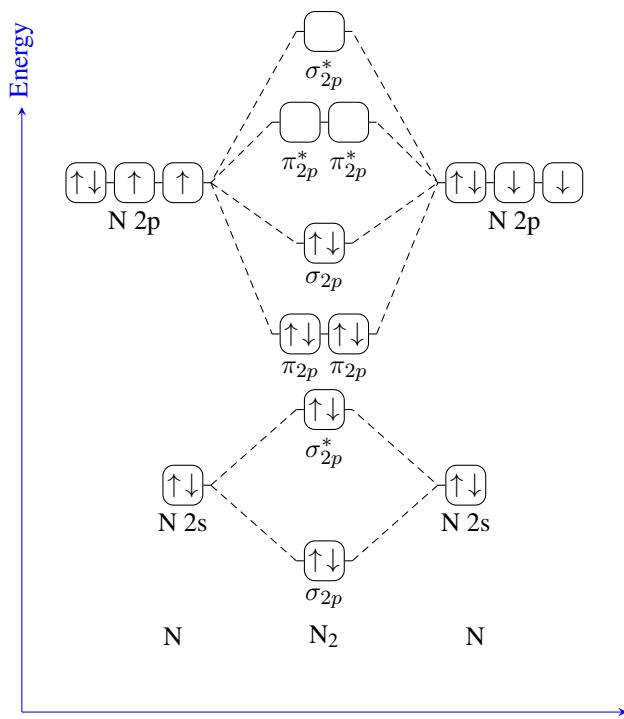
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From MO diagram to MO configuration Obtaining a MO diagram is not obvious, and these diagrams can only be obtained after very complicated quantum mechanics simulations. However, after the MO diagram is given, one can obtain the MO configuration. From 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 N₂:



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In this diagram, the lower MO's are the most stables and should be filled first. The higher MO are less stable and they are listed in the right side of the MO configuration. For example, the MO configuration of N_2 would be:

$$\text{N}_2 = \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$$

Bond order of a MO configuration Lets go back to the MO configuration for N_2 . In this configuration we have some of the electrons occupying bonding MO and other 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:

$$BO = \frac{(n - n^*)}{2}$$

Bond Order

where:

n is the number of electrons occupying bonding MO's

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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 more loose.

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Sample Problem 104

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 $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2$.

Answer: 3.

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Paramagnetism and diamagnetism We can also predict the magnetic character of a molecule by means of the MO configuration. Paramagnetic molecules are attracted by magnetic fields, whereas diamagnetic molecules are repelled by magnetic fields. The paramagnetic character is due to the presence of unpaired electrons. For example: $\sigma_{2s}^2 \sigma_{2s}^{*1}$ is a paramagnetic molecule as we have one unpaired electron in the σ_{2s}^* orbital. Differently, $\sigma_{2s}^2 \sigma_{2s}^{*2}$ is a diamagnetic molecule, as it has no unpaired electrons.

Sample Problem 105

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) $\sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^4 \sigma_{2p}^2 \pi_{2p}^{*2}$.

Answer: both diamagnetic.

CHAPTER 10

ELECTRON-DOT STRUCTURES OF MOLECULES

10.1 Draw the electron-dot structure of: (a) BH_3
(b) CH_4

10.2 Draw the electron-dot structure of: (a) NH_4^+
(b) H_3O^+

10.3 The electron-dot structure of HI is:

- (a) $\underline{\text{H}} - \underline{\text{I}}$ (d) $\bar{\text{H}} - \bar{\text{I}}$
 (b) $\underline{\text{H}} - \overline{\text{I}}$ (e) $\text{H} - \overline{\text{I}}$
 (c) $\overline{\text{H}} - \underline{\text{I}}$

10.4 Indicate the charge of the central atom in the following electron-dot structure:

- (a) $\left[\begin{array}{c} \text{H} - \overset{\circ}{\text{C}} - \text{H} \\ | \\ \text{H} \end{array} \right]$ (b) $\left[\begin{array}{c} \text{H} - \overset{\circ}{\text{O}} - \text{H} \\ | \\ \text{H} \end{array} \right]$

10.5 Indicate the charge of the central atom in the following electron-dot structure:

- | | | | |
|-----|--|-----|--|
| (a) | $\left[\begin{array}{c} \text{H} \\ \\ \text{H}-\text{N}-\text{H} \\ \\ \text{H} \end{array} \right]$ | (b) | $\left[\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{O} \\ \\ \text{H} \end{array} \right]$ |
|-----|--|-----|--|

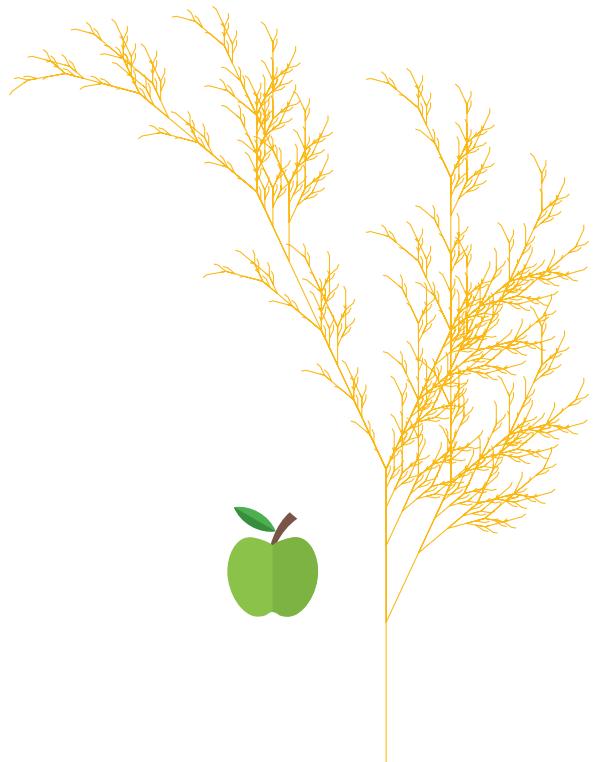
MOLECULAR SHAPE

10.6 Identify the molecular shape of the molecules:
 NH_3 CH_4

10.7 Identify the molecular shape of the molecules:
 (a) H₂ (b) BeCl₂ BF₃

POLARITY

Answers **10.1** (a) H—B—H (b) H—C—H **10.3** H— $\overline{\text{I}}$ **10.5** (a) +1 (b) -1 **10.7** (a) H₂ (Linear) (b) BeCl₂ (Linear) BF₃ (Trigonal planar) **10.9** (a) NH₃ (b) CO₂ **10.11** (a) NH₃ (sp^3) (b) CH₄ (sp^3) (c) H₂O (sp^3) **10.13** (a) O₂ ($\sigma_{2s}^2 \sigma_{2s}^{2*} \sigma_{2p}^2 \pi_{2p}^4 \pi_{2p}^{2*}$) (b) F₂⁺ ($\sigma_{2s}^2 \sigma_{2s}^{2*} \sigma_{2p}^2 \pi_{2p}^4 \pi_{2p}^{3*}$)



College Chemistry

A Comprehensive Set of Imperfect Notes

This set of lectures intend to cover the first semester of a College Chemistry class. The intention here is to present the 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 as well as a periodic table. The organization of the notes is based on 10 chapters and five parts, each made of two chapters. This organization is intended to help the reader digest the large content typically covered in a General Chemistry class. Every part ends with a review quiz that assesses content. Finally, this set of notes are made to complement and not replace any existing textbook.