College Of Engineering University Of Anbar



Dept. of Chem. & Petrochemical Engineering Subject : Chemistry First Stage

Lecture 1

MEASUREMENTS IN CHEMISTRY

2022 – 2023



- **1.1** Units of Measurement
- **1.2** Scientific Notation
- **1.3** Metric Prefixes
- **1.4** Significant Figures in Measurements
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MEASUREMENTS IN CHEMISTRY

- Measurements are part of our daily lives. We measure our weights, driving distances, and gallons of gasoline. As a health professional you might measure blood pressure,
- temperature, pulse rate, drug dosage, or percentage of body fat.
- A **measurement** contains a *number* and a *unit*.
- A *unit* specifies the physical property and the size of a measurement, while the *number* indicates how many units are present. A number without a unit is usually meaningless.

1.1 Units of Measurement

In the United States most measurements are made with the English system of units which usually contain fractions (a collection of functionally unrelated units.) The metric system is a decimal-based system of units of measurement which is used most often worldwide.

Around 1960, the international scientific organization adopted a modification of the metric system called **International System or SI** (from System International).

Quantity	English Unit	Metric Unit	SI Unit
Mass	pound (lb)	gram (g)	kilogram (kg)
Length	foot (ft)	meter (m)	meter (m)
Volume	quart (qt)	liter (L)	cubic meter (m ³)
Temperature	degree Fahrenheit (°F)	degree Celsius (°C)	Kelvin (K)
Energy	calorie (cal)	calorie (cal)	Joule (J)

1.2 Scientific Notation

Scientific notation is a common method used to represent very small or very large numbers conveniently. There are two parts to any number expressed in scientific notation, a **coefficient**, and a power of 10. The number 683 is written in scientific notation as 6.83×10^2 .

The coefficient is 6.83 and 10^2 shows the power of 10 (the superscript 2 is called an **exponent**). A number less than one would contain a negative exponent. For example: the number 0.0075 is written as 7.5 x 10^{-3} (note the negative exponent).

The **coefficient** must always be a number **greater than or equal to 1** but **less than 10** or 1 coefficient < 10.

Worked Example 1-1

Express the following numbers in scientific notation: a) 408.00 b) 0.007956

Solution

Apply the following:

Place the decimal point after the first nonzero digit in the number.

Indicate the number of places the decimal was moved using the power of 10. If the decimal is moved to the left, the power of 10 is positive. If moved to the right, it is negative.

a) $4.0800 \ge 10^2$ (coefficient = 4.0800, exponent = +2) b) $7.956 \ge 10^{-3}$ (coefficient = 7.956, exponent = -3)

Practice 1-1

Express each of the following values in scientific notation:

- a) There are 33,000,000,000,000,000,000 molecules of water in one milligram of water.
- b) A single molecule of sucrose weighs 0.000 000 000 000 000 000 000 57 g.

Answer

```
a) 3.3 x 10<sup>19</sup> (coefficient = 3.3, exponent = 19)
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b) 5.7 \ge 10^{-22} (coefficient = 5.7, exponent = -22)
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Practice 1-2

Convert each the following scientific notation to decimal notation.

a) 8.54×10^3 b) 6.7×10^{-5} c) 1.29×10^4 d) 1.000×10^{-2}

Answer



Scientific Notation and Calculators

Numbers in scientific notation can be entered into most calculators using the EE or EXP key. As an example try 9.7×10^3 .

- 1. Enter the coefficient (9.7) into calculator.
- 2. Push the EE (or EXP) key. Do NOT use the x (times) button.

3. Enter the exponent number (3).

Number to Enter	Method	Display Reads
9.7 x 10 ³	9.7 EE or EXP 3	9.7 ⁰³ or 9.7E03 or 9700

Now try $8.1 \ge 10^{-5}$:

- 1. Enter the coefficient (8.1) into calculator.
- 2. Push the EE (or EXP) key. Do NOT use the x (times) button.
- 3. Enter the exponent number (5). Use the plus/minus (+/-) key to change its sign.

Number to Enter	Method	Display Reads
8.1 x 10 ⁻⁵	8.1 EE or EXP 5 +/-	8.1 ⁻⁰⁵ or 8.1E-05

1.3 Metric Prefixes

The metric system is a decimal-based system of units of measurement used by most scientists worldwide.

In the metric system, a prefix can be attached to a unit to increase or decrease its size by factors (powers) of 10.

	Prefix	Value
Î	tera- (T) giga- (G) mega- (M) kilo- (k)	$10^{12} = 1,000,000,000,000$ $10^{9} = 1,000,000,000$ $10^{6} = 1,000,000$ $10^{3} = 1,000$
	deci- (d) centi- (c) milli- (m) micro- (µ) nano- (n) pico- (p)	$10^{-1} = 0.1$ $10^{-2} = 0.01$ $10^{-3} = 0.001$ $10^{-6} = 0.000001$ $10^{-9} = 0.000000001$ $10^{-12} = 0.00000000001$

Practice 1-3

Give the metric prefix that corresponds to each of the following a) 1,000,000,000 b) 10^{-6} c) 1000 d) 0.01 e) 10^{-9} f) 10^{12}

Answer

a) giga	b) micro	c) kilo	
d) centi	e) nano	f) tera	

1.4 Significant Figures in Measurements

- A student is asked to determine the mass of a small object using two different balances available in the lab. The lower priced model reports masses to within ±0.01 g (one-one hundredth), while the higher priced one reports to within ±0.0001 g (one-ten thousandth).
- The student measures the mass three times on each balance and completes the following table.

	First balance	Second balance
Three measurements	2.16, 2.14, 2.15 g	2.1538, 2.1539, 2.1537 g
Average	2.15 g	2.1538 g
Reproducibility	±0.01 g	±0.0001 g
Which digit is the "uncertain digit" in the average?	The last digit; 5	The last digit; 8
Which digits are "certain digits" in the average?	2, 1	2, 1, 5, 3
How many significant digits are in the average?	Three significant digits	Five significant digits

• Significant figures (sig figs) are the digits that are known with certainty plus one digit that is uncertain. All nonzero digits in measurements are always significant.

• Are zeroes significant?

- **YES:** zeros between nonzero digits (20509).
- **YES:** zeros at the end of a number when a decimal point is written (3600.).
- NO: zeros at the end of a number when no decimal point is written (3600).
- NO: zeros at the beginning of a number (0.0047).

Worked Example 1-2

How many significant figures does each number have?

a) 0.0037	b) 600.	c) 93,000
d) 2.08 x 10 ⁻⁵	e) 600	f) 58.00
g) 4010049	h) 1.700 x 10 ²	i) 4.0100 x 10 ⁶

Solution

	sf		sf		sf
0.0037	2	600.	3	93,000	2
2.08 x 10 ⁻⁵	3	600	1	58.00	4
4010049	7	$1.700 \ge 10^2$	4	$4.0100 \ge 10^6$	5

Significant Figures in "Exact Numbers"

- Exact numbers have an **unlimited** number of significant figures. Exact numbers are obtained by **counting** items or by **definition**.
- Counting: 24 students mean 24.0000000... students. 8 pennies means 8.0000... pennies.
- Definition: 1 m = 100 cm means 1.00000....m = 100.000000....cm

Example for lecture -1 What are the significant figures rules?

- To determine what numbers are significant and which aren't, use the following rules:
- 1. The zero to the left of the decimal value less than 1 is not significant.
- 2. A final zero or trailing zeros in the decimal portion <u>ONLY</u> are significant.
- 3. Zeros between non zero numbers are significant.
- 4. All non zero numbers are significant.
- If a number has more numbers than the desired numbers of significant digits, the number is rounded. For example, 432,500 is 433,000 to 3 significant digits.
- Zeros at the end of numbers which are not significant but are not removed, as removing would affect the value of the number. In the above example, cannot remove 000 in 432, 000 unless changing the number into scientific notation.

- Rule 1: Non-zero digits are always significant.
- Hence a number like 26.38 would have four significant figures and 7.94 would have three.
 The problem comes with numbers like 0.00980 or 28.09.

Rule 2: Any zeros between two significant digits are significant.

Suppose you had a number like 406. By the first rule, the 4 and the 6 are significant. [However, to make a measurement decision on the 4 (in the hundred's place) and the 6 (in the unit's place), you HAD to have made a decision on the ten's place. The measurement scale for this number would

have hundreds and tens marked with an estimation made in the unit's place. Like this:



- Rule 3: A final zero or trailing zeros in the decimal portion <u>ONLY</u> are significant.
- This rule causes the most difficulty with students. Here are two examples of this rule with the zeros this rule affects in boldface:
 - 0.00500
 - 0.0304**0**
- Here are two more examples where the significant zeros are in boldface:
 - 2.30×10^{-5}
 - 4.500×10^{12}

What Zeros are Not Discussed Above

Zero Type #1: Space holding zero on numbers less than one.

Here are the first two numbers from just above with the digits that are NOT significant in boldface:

0.00500

0.03040

These zeros serve only as space holders. They are there to put the decimal point in its correct location. They DO NOT involve measurement decisions. Upon writing the numbers in scientific notation $(5.00 \times 10^{-3} \text{ and } 3.040 \times 10^{-2})$, the non-significant zeros disappear.

Zero Type #2: the zero to the left of the decimal point on numbers less than one.

When a number like 0.00500 is written, the very first zero (to the left of the decimal point) is put there by convention. Its sole function is to communicate unambiguously that the decimal point is a deciaml point. If the number were written like this, .00500, there is a possibility that the decimal point might be mistaken for a period. Many students omit that zero. They should not.

Zero Type #3: trailing zeros in a whole number.

- 200 is considered to have only ONE significant figure while 25,000 has two.
- This is based on the way each number is written. When whole number are written as above, the zeros, BY DEFINITION, did not require a measurement decision, thus they are not significant.
- However, it is entirely possible that 200 really does have two or three significant figures. If it does, it will be written in a different manner than 200.
- Typically, scientific notation is used for this purpose. If 200 has two significant figures, then 2.0 x 10² is used. If it has three, then 2.00 x 10² is used. If it had four, then 200.0 is sufficient.

See rule #2 above.

How will you know how many significant figures are in a number like 200? In a problem like below, divorced of all scientific context, you will be told. If you were doing an experiment, the context of the experiment and its measuring devices would tell you how many significant figures to report to people who read the report of your work.

Zero Type #4: leading zeros in a whole number. 00250 has two significant figures. 005.00 x 10⁻4 has three.

1.5 Calculations Involving Significant Figures

Rules for Rounding off Numbers If the first digit to be deleted is 4 or less, leave the last reported digit unchanged.

If the first digit to be deleted is 5 or greater, increase the last reported digit by one.

In some cases you need to add significant zeros. The number 2, reported in four significant figures, is 2.000.

Prac	Round off each of the a) 9.174 d) 5	e following to b) 9.175 e) 0.0040	three significant f c) 9.176 f) 8000	igures.
Answ	g) 2.4 x 10 ⁻⁵ er a) 9.174 (9.17)	h) 670 b) 9.	175 (9.18)	c) 9.176 (9.18)
	d) 5 (5.00) g) 2.4 x 10 ⁻⁵ (2.40	e) 0. x 10⁻⁵) h) 67	0040 (0.00400) 70 (670.)	f) 8000 (8.00 x 10 ³)
	g) 211 II 10 (2110	110 <i>J</i> 1)01		

Rules for Rounding off in Calculations A. Multiplication and Division

The answer carries the **same number of significant figures** as the factor with the fewest significant figures

Practice 1-5

 Perform each of the following calculations to the correct number of significant figures.

 a) $33.56 \ge 1.9483$ b) $(2.50 \ge 10^{-3}) \ge (1.8500 \ge 10^{5})$

 c) $47.5301 \div 2.30$ d) $(6.56 \ge 10^{10}) \div (7.8 \ge 10^{9})$

Answer

a) $33.56 \ge 1.9483 = 65.38$ b) $(2.50 \ge 10^{-3}) \ge (1.8500 \ge 10^{5}) = 4.63 \ge 10^{2}$ c) $47.5301 \div 2.30 = 20.7$ d) $(6.56 \ge 10^{10}) \div (7.8 \ge 10^{9}) = 8.4$

B. Addition and Subtraction

The answer should have the **same number of decimal places** as the quantity with the fewest decimal places.

Practice 1-6

Perform each of the following calculations to the correct number of significant figures:

a) 73.498 + 2.2 c) 191.000 - 188.0

e)
$$(6.8 \times 10^{-2}) + (2.04 \times 10^{-2})$$

b) 63.81 + 205.4 d) 124.08 - 39.1740 f) (5.77 x 10⁻⁴) - (3.6 x 10⁻⁴)

Answer

a) 73.498 + 2.2 = 75.7	b) $63.81 + 205.4 = 269.2$
(-) 101 000 188 0 $-$ 2 0	$\frac{1}{124.09} = 20.1740 - 94.01$
c) $191.000 - 188.0 = 3.0$	a) $124.08 - 39.1740 = 84.91$
e) $(6.8 \times 10^{-2}) + (2.04 \times 10^{-2}) =$ 8.8 x 10^{-2}	t) $(5.77 \times 10^{-4}) - (3.6 \times 10^{-4}) =$ 2.2 × 10 ⁻⁴
0.0 X 10	2.2 X 10

Question 1 How many significant figures are in the following values? a. 4.02 x 10-9 b. 0.008320 • c. 6 x 105 d. 100.0

Question 2 How many significant figures are in the following values? a. 1200.0 b. 8.00 c. 22.76 x 10-3 d. 731.2204

Question 3 Which value has more significant figures? 2.63 x 10-6 or 0.0000026

Question 4 Express 4,610,000 in scientific notation. a. with 1 significant figure b. with 2 • significant figures c. with 3 significant figures d. with 5 significant figures

Question 5 Express 0.0003711 in scientific notation. a. with 1 significant figure b. with 2 significant figures c. with 3 significant figures d. with 4 significant figures

Question 6 Perform the calculation with the correct number of significant digits. 22.81 + • 2.2457

Question 7 Perform the calculation with the correct number of significant digits. 815.991 x • 324.6

Question 8 Perform the calculation with the correct number of significant digits. 3.2215 + 1.67 + 2.3

Question 9 Perform the calculation with the correct number of significant digits.8.442 - 8.429Question 10 Perform the calculation with the correct number of significant digits.27/3.45

Answers 1. a. 3 b. 4 c. 1 d. 4 2. a. 5 b. 3 c. 4 d. 7 3. 2.63 x 10-6 •

4. a. 5 x 106 b. 4.6 x 106 c. 4.61 x 106 d. 4.6100 x 106 **5.** a. 4 x 10-4 •

b. 3.7 x 10-4 c. 3.71 x 10-4 d. 3.711 x 10-4 **6.** 25.06 **7.** 2.649 x 105 **• 8.** 7.2 **9.** 0.013 **10.** 7.8 **•**

1.6 Writing Conversion Factors

Many problems in chemistry require converting a quantity from one unit to another. To perform this conversion, you must use a conversion factor or series of conversion factors that relate two units. This method is called dimensional analysis. Any equality can be written in the form of a fraction called a conversion factor. A conversion factor is easily distinguished from all other numbers because it is always a fraction that contains different units in the numerator and denominator. Converting kilograms to pounds can be performed using the equality 1 kg = 2.20 lb. The two different conversion factors that may be written for the equality are shown below. Note the different units in the numerator and denominator, a requirement for all conversion factors.

Conversion Factors:
$$\frac{\text{Numerator}}{\text{Denominator}}$$
 $\frac{1 \text{ kg}}{2.20 \text{ lb}}$ or $\frac{2.20 \text{ lb}}{1 \text{ kg}}$

Some common units and their equivalents are listed in Table 1.1. You should be able to use the information, but you will **not** be responsible for memorizing the table. The Table will be given to you during quizzes and exams.

Table 1.1 Some Common Units and Their Equivalents

Length	1 m = 100 cm	1 m = 1000 mm	1 cm = 10 mm	1 km = 1000 m	1nm = 10 ⁻⁹ m
	$1 \text{\AA} = 10^{-10} \text{ m}$	1 in = 2.54 cm	1 ft = 30.48 cm	1 mi = 1.61 km	1 yd = 0.91 m
	1 ft = 12 in.				
Mass	1 kg = 1000 g	1 g = 1000 mg	1 lb = 454 g	1kg = 2.20 lb	1 oz = 28.35 g
	1 lb = 16 oz				
Volume	1L = 1000 mL	$1 \text{ mL} = 1 \text{ cm}^3$	1qt = 0.946 L	1 gal = 3.78 L	
Energy	1 cal = 4.18 J				
Temperature	°F = 1.8°C + 32	°C = (°F -32)/1.8	K = °C + 273.15		

	Metric to English	English to Metric
Length		
1.00 inch $= 2.54$ continuators	1.00 in.	2.54 cm
1.00 men - 2.34 centimeters	2.54 cm	1.00 in.
1.00 meter = 30.4 inches	39.4 in.	1.00 m
1.00 meter -39.4 menes	1.00 m	39.4 in.
1.00 kilomator = 0.621 milo	0.621 mi	1.00 km
1.00 knometer -0.021 mile	1.00 km	0.621 mi
Mass		
1.00 nound = 454 arrange	1.00 lb	454 g
1.00 pound = 434 grains	454 g	1.00 lb
1.00 kilogram = 2.20 pounds	2.20 lb	1.00 kg
1.00 knogram = 2.20 pounds	1.00 kg	2.20 lb
1.00 output = 28.3 grams	1.00 oz	_28.3 g
1.00 ounce – 28.5 grams	28.3 g	1.00 oz
Volume		
1.00 quart = 0.046 liter	1.00 qt	0.946 L
1.00 quart = 0.940 mer	0.946 L	1.00 qt
1.00 liter = 0.265 caller	0.265 gal	1.00 L
1.00 liter = 0.205 gallon	1.00 L	0.265 gal
1.00 millilitor = 0.024 fluid our co	0.034 fl oz	1.00 mL
1.00 minimiter – 0.054 multi ounce	1.00 mL	0.034 fl oz

Worked Example 1-3

Write conversion factors for each of the following equalities or statements:

- a) 1 g = 1000 mg
- c) 1 quart = 0.946 liter

b) 1 foot = 12 inches

d) The accepted toxic dose of mercury is 0.30 mg per day.

Solution

Equality	Conversion factor	Conversion factor
1 g = 1000 mg	1 g 1000 mg	<u>1000 mg</u> 1 g
1 foot = 12 inches	$\frac{1 \text{ ft.}}{12 \text{ in.}}$	<u>12 in.</u> 1 ft.
1 quart = 0.946 liter	1 qt. 0.946 L	0.946 L 1 qt.
The accepted toxic dose of mercury is 0.30 mg per day.	0.30 mg 1 day	1 day 0.30 mg

1.7 Problem Solving in Chemistry - Dimensional Analysis

Dimensional analysis is a general method for solving numerical problems in chemistry. In this method we follow the rule that when multiplying or dividing numbers, we must also multiply or divide units.

Solving problems by dimensional analysis is a three-step process:

1. Write down the given measurement; number with units.

2. Multiply the measurement by one or more conversion factors. The unit in each denominator must cancel (match) the preceding unit in each numerator.

3. Perform the calculation and report the answer to the proper significant figures based on numbers given in the question (data), not conversion factors used.

Worked Example 1-4

Convert 0.455 km to meters.

Solution

To convert kilometers to meters, we could use the following equality: 1 km = 1000 m (See Table 1.1)

The corresponding conversion factors would be:

1 km	and	1000 m
1000 m	anu	1 km

We select the conversion factor to cancel kilometers, leaving units of meters.

$$0.455 \text{ km} = 455 \text{ m}$$

The number of significant figures in your answer reflect 0.455 km. The exact conversion factor does not limit the number of significant figures in your answer.

Worked Example 1-5

Convert 4.5 weeks to minutes.

Solution



Worked Example 1-6

Convert 2.7 g/mL to lb/L.

Solution

We need two conversion factors: one to convert g to lb and the other to convert mL to L. We know that 1 lb= 454 g and 1 L = 1000 mL (See Table 1.1)

 $\frac{2.7 \text{ y}}{1.0 \text{ mL}} = 5.9 \text{ lb/L}$ Remember that the number of significant figures in your answer reflect 2.7. The conversion factors do not limit the number of significant figures in your answer.

Practice 1-7

Perform each of the following conversions:

a) Convert 14.7 lb to ounces. b) Convert 19.8 lb to kilograms.

c) Convert 23 m/sec to mi/hr.

Answer



1.8 Density and Specific Gravity

Density is the ratio of the mass of a substance to the volume occupied by that substance.

density =
$$\frac{\text{mass of substance}}{\text{volume of substance}}$$
 or $d = \frac{m}{V}$

Density is expressed in different units depending on the phase (form) of the substance. Solids are usually expressed in grams per cubic centimeter (g/cm_3), while liquids are commonly grams per milliliter (g/mL). The density of gases is usually expressed as grams per liter (g/L)

Worked Example 1-7

If 10.4 mL of a liquid has a mass of 9.142 g, what is its density?

Solution

$$d = \frac{m}{V}$$
 $d = \frac{9.142 \text{ g}}{10.4 \text{ mL}} = 0.879 \text{ g/mL}$

Density can be used as a conversion factor that relates mass and volume, note the different units in the numerator and denominator. Densities can be used to calculate mass if volume is given or calculate volume given mass. For example, we can write two conversion factors for a given density of 1.05 g/mL:

$$\frac{1.05 \text{ g}}{1.00 \text{ mL}}$$
 or $\frac{1.00 \text{ mL}}{1.05 \text{ g}}$

Worked Example 1-8

The density of a saline solution is 1.05 g/mL. Calculate the mass of a 377.0 mL sample.

Solution

 $d = \frac{m}{V}$ m = 377.0 mL x $\frac{1.05 g}{1.00 mL}$ = 396 g

Practice 1-8

The density of rubbing alcohol is 0.786 g/mL. What volume of rubbing alcohol would you use if you needed 32.0 g?

Answer

We use the density as a conversion factor: 1.00 mL V = 32.0 g x = 40.7 mL 0.786 g **Specific Gravity** is the ratio of the density of liquid to the density of water at 4°C, which is 1.00 g/mL. Since specific gravity is a ratio of two densities, the units cancel.

specific gravity =
$$\frac{\text{density of sample (g/mL)}}{\text{density of water (g/mL)}}$$
 (No units)

An instrument called a *hydrometer* is used to measure the specific gravity of liquids.

Worked Example 1-9

What is the specific gravity of jet fuel if the density is 0.775 g/mL?

Solution

specific gravity = $\frac{0.775 \text{ g/mL}}{1.00 \text{ g/mL}} = 0.775$

Practice 1-9

A 50.0 mL sample of blood has a mass of 53.2 g.

- a) Calculate the density of the blood.
- b) Calculate the specific gravity of the blood.

Answer

d = V	a) $d = {53.2 \text{ g} \over 50.0 \text{ mL}} = 1.06 \text{ g/mL}$	
specific gravity =	density of blood 1.06 g/mL = 1.00 g/mL	= 1.06
1.9 Temperature Scales

Temperature, reported in Fahrenheit (°F) or Celsius (°C), is used to indicate how hot or cold an object is. The SI unit for reporting temperature is Kelvin (K)

See the comparison of the three scales:

	Freezing point of water	Boiling point of water	Normal body temperature
Fahrenheit	32°F	212°F	98.6°F
Celsius	0°C	100°C	37°C
Kelvin	273 K	373 K	310 K

The following formulas show the conversions:

Fahrenheit to Celsius:
$$^{\circ}C = \frac{(^{\circ}F - 32)}{1.8}$$

Celsius to Fahrenheit: $^{\circ}F = 1.8 \ ^{\circ}C + 32$

Celsius to Kelvin: K = °C + 273

Practice 1-10

Fahrenheit	Celsius	Kelvin
88°F		
	-55°C	
		469K

Complete the following table.

Fahrenheit	Celsius	Kelvin
88°F	31°C	304 K
-67°F	-55°C	218 K
385°F	196°C	469 K

1.10 Heat and Specific Heat

Heat and temperature are both a measure of energy. Heat, however, is not the same as temperature. Heat measures the total energy, whereas temperature measures the average energy. A gallon of hot water at 200 F has much more heat energy than a teaspoon of hot water at same temperature. Heat can be measured in various units. The most commonly used unit is calorie (cal). The calorie is defined as the amount of heat required to raise the temperature of 1 gram of water by 1°C. This is a small unit, and more often we use kilocalories (kcal).

1 kcal = 1000 cal

Nutritionist use the word "Calorie" (with a capital "C") to mean the same thing as kilocalorie.

1 Cal = 1000 cal = 1 kcal

The unit of energy in SI unit is **joule** (pronounced "jool"), which is about four times as big as the calorie:

$$1 \text{ cal} = 4.184 \text{ J}$$

- How to convert joules to calories
- How to convert energy in joules (J) to calories (cal).
- Small & large calories
- *Small calorie* (cal) is the energy needed to increase 1 gram of water by 1°C at a pressure of 1 atmosphere.
- Large calorie (Cal) is the energy needed to increase 1 kg of water by 1°C at a pressure of 1 atmosphere.
- Large calorie is also called food calorie and is used as a unit of food energy.
- How to convert from joules to calories
- Joules to thermochemical calories
- $1 \operatorname{cal}_{\mathrm{th}} = 4.184 \mathrm{J}$
- The energy in thermochemical calories $E_{(calth)}$ is equal to the energy in joules $E_{(J)}$ divided by 4.184:
- $E_{(cal)} = E_{(J)} / 4.184$
- Example
- Convert 600 joules to thermochemical calories.
- $E_{(cal)} = 600 \text{J} / 4.184 = 143.4 \text{ cal}_{th}$
- Joules to 15°C calories
- $1 \operatorname{cal}_{15} = 4.1855 \operatorname{J}$
- The energy in 15°C calories $E_{(cal15)}$ is equal to the energy in joules $E_{(J)}$ divided by 4.1855:
- $E_{(cal15)} = E_{(J)} / 4.1855$
- Example
- Convert 600 joules to 15°C calories.
- $E_{(cal15)} = 600 \text{J} / 4.1855 = 143.352 \text{ cal}_{15}$

Specific Heat

Substances change temperature when heated, but not all substances have their temperature raised to the same extent when equal amounts of heat are added.

Specific Heat is the amount of heat required to raise the temperature of one gram of a substance by one degree Celsius. It is measured in units of cal/g·°C or J/g·°C.

(Recall; 1 cal is required to raise the temperature of 1 gram of water by 1°C, the specific heat of water is therefore: 1.00 cal/g·°C, or 4.184 J/g·°C).

Specific heats for some substances in various states are listed in the following table. A substance with a high specific heat is capable of absorbing more heat with a small temperature change than a substance with lower specific heat.

	Substance	Specific Heat (J/g·°C)
Solids		
201100	gold	0.128
	copper	0.385
	aluminum	0.903
	ice	2.06
Liquids		
-	mercury	0.138
	methanol	1.77
	ethanol	2.42
	water	4.18
Gases		
	argon	0.518
	oxygen	0.915
	nitrogen	1.041
	steam	2.03

Specific Heats for Some Common Substances

We can calculate the amount of heat gained or lost by a substance using its specific heat, its measured mass, and the temperature change.

Amount of heat	t =	mass	х	specific heat	х	change in temperature*
q	=	m	х	SH	х	$(T_{final} - T_{initial})$

* The temperature change could also be written as Δ (*delta* T).

If any three of the four quantities in the equation are known, the fourth quantity can be calculated.

Worked Example 1-10

Determine the amount of heat that is required to raise the temperature of 7.400 g of water from 29.0°C to 46.0°C. The specific heat of water is 4.18 J/g·°C.

Solution

 $q = m x SH x \Delta T$ $q = 7.400 g x 4.18 J/g \cdot C x 17.0 C = 526 J$

Practice 1-11

What mass of lead is needed to absorb 348 J of heat if the temp of the sample rises from 35.2°C to 78.0°C? The specific heat of lead is 0.129 J/g·°C.



Practice 1-12

It takes 87.6 J of heat to raise the temp of 51.0 g of a metal by 3.9°C. Calculate the specific heat of the metal.

$\mathbf{q} = \mathbf{m} \mathbf{x} \mathbf{S} \mathbf{H} \mathbf{x} \Delta \mathbf{T}$				
so SH :	q =			
	m x ∆T			
с н –	87.6 J	-0.44 $I/\sigma^{0}C$		
511 =	51.0 g x 3.9°C	– 0.44 J/g°C		

Practice 1-13

 4.00×10^3 J of energy is transferred to 56.0 g of water at 19°C. Calculate the final temperature of water. SH = $4.18 \text{ J/g} \cdot ^{\circ}\text{C}$.



Homework Problems

1.1 Complete the following table.

Decimal notation	Scientific notation	Number of significant figures
400,000		
0.000600		
21,995,000		
0.05050		
	$7.28 \ge 10^3$	
	3.608 x 10 ⁻⁵	
	9.4090 x 10 ⁴	
	1.5 x 10 ⁻³	

1.2 Perform the following calculations to correct number of significant figures.

a. $4.6 \ge 0.00300 \ge 193$ b. $8.88 \div 99.40$ c. $(7.120 \ge 10^{-3}) \div (6.000 \ge 10^{-5})$ d. $(5.92 \ge 10^3) \ge 3.87 \div 100$ 1.3 Perform the following calculations to correct number of significant figures.

a. 102 - 5.31 - 0.480b. $(3.42 \times 10^{-4}) + (5.007 \times 10^{-4})$ c. $7.8 - (8.3 \times 10^{-2})$ d. $(3.8 \times 10^{6}) - (8.99 \times 10^{6})$

1.4 Perform the following conversions. Show your set ups.

a. 683 nanometer (nm) to angstrom (Å)
b. 520 mi/h to m/sec
c. 0.714 g/cm₃ to lb/ft₃
d. -164°C to °F

1.5 A physician has ordered 37.5 mg of a particular drug over 15 minutes. If the drug was available as 2.5 mg/mL of solution, how many mL would you need to give every 15 seconds? 1.6 What is the density of a metal sample if a15.12-g sample is added into a graduated cylinder increased the liquid level from 35.00 mL to 40.60 mL?

1.7 The density of copper is 8.96 g/cm₃. You have three different solid samples of copper. One is **rectangular** with dimensions 2.3 cm x
3.1 cm x 8.0 cm. The second is a **cube** with edges of 3.8 cm. The third is a **cylinder** with a radius of 1.5 cm and a height of 8.4 cm. Calculate the mass of each sample

1.8 A 50.00-g sample of metal at 78.0°C is dropped into cold water. If the metal sample cools to 17.0°C and the specific heat of metal is $0.108 \text{ cal/g} \cdot ^{\circ}\text{C}$, how much heat is released?

ANY QUESTIONS??





College Of Engineering

University Of Anbar





Dept. of Chem. & Petrochemical Engineering Subject : Chemistry First Stage

Lecture 3

Atoms, Molecules and Ions



Lecturer Dr. Mohamad Jasim

2022-2023

Lecture Outline

- 2.1 The Atomic Theories
- 2.2 The structure of the atom
- 2.3 Atomic number, mass number and isotopes
- 2.4 The periodic table
- 2.5 Molecules and ions
- 2.6 Chemical formula
- 2.7 Naming compounds

THE EVOLUTION OF THE ATOMIC MODEL

Dalton's Atomic Theory

- 1. Elements are composed of extremely small particles called *atoms*. *Atoms* of the same element all have the same size, mass, and chemical properties. The atoms of one element are different from the atoms of all other elements.
- 2. Compounds are composed of atoms of two or more elements. In any compound, the ratio of the numbers of atoms of any two of the elements present is either an integer or a simple fraction.
- 3. A *chemical reaction* involves only the separation, combination, or rearrangement of atoms; it does not result in their creation or destruction.

atom of the element oxygen



An atom of the elem

oms of a given element are identical, but the atoms of one e fferent from the atoms of all other elements.





s of one element cannot be changed into atoms of a differer emical reactions; atoms are neither created nor destroyed ir ons.



 Compounds are formed when atoms of mo element combine; a given compound alway same relative number and kind of atoms.

Dalton's Atomic Theory





Law of Definite Proportions

-Different samples of the same compound always contain their elements in a definite proportion by mass.

-Compounds contain fixed proportions of their constituent elements. These proportions do not change, regardless of the different methods of preparing the compound.

Dalton's Atomic Theory



Law of Multiple Proportions

-In different compounds of the same elements, the various masses of one element that combine with a fixed mass of another element are related by small whole-number ratios.

Dalton's Atomic Theory



Atoms of element X







Compounds of elements X and Y



Law of Conservation of Mass

- Matter is neither created nor destroyed

The Modern View of Atomic Structure

Atom- the basic unit of an element that can enter into chemical combination (extremely small and indivisible)

Three **subatomic particles** - electrons , protons, and neutrons.

Thomson Cathode Ray Tube experiment



- The cathode ray consist of negatively charged particles found in all matter
- Thomson together with Millikan concluded that the mass of an e- is exceedingly small (e⁻ mass = 9.10×10^{-28} g).



Three types of rays produced by decay of radioactive substances such as "Uranium"..

(i) Alpha (α) rays..positively charged particles (α) particles.. deflected by positively charged plate

(ii) Beta (β) rays..electrons..deflected by negatively charged plate

(iii) Gamma (γ) rays..high-energy rays..no charge and are not affected by an external field.

Thomson's Model

a spherical atom
composed of diffuse,
positively charged matter, in
which e- is embedded like a
"raisin in a plum pudding".

Thompson plum pudding model of the atom





Rutherford's gold foil α -scattering experiment



Atoms of gold foil

Ernest Rutherford Model: Rutherford discovered the nucleus of the atom in 1911



Rutherford's Model of the Atom

- 1. atoms positive charge is concentrated in the nucleus
- 2. proton (p) has opposite (+) charge of electron (-)
- 3. mass of p is 1840 x mass of e^{-1} (1.67 x 10⁻²⁴ g)



atomic radius ~ 100 pm = 1 x 10^{-10} m

nuclear radius ~ $5 \times 10^{-3} \text{ pm} = 5 \times 10^{-15} \text{ m}$

Chadwick's Experiment (1932)



neutron (n) is neutral (charge = 0) n mass ~ p mass = $1.67 \times 10^{-24} \text{ g}$

TABLE 2.1 Mass and Charge of Subatomic Particles

Particle		Char	ge
	Mass (g)	Coulomb	Charge Unit
Electron*	9.10938×10^{-28}	-1.6022×10^{-19}	-1
Proton	1.67262×10^{-24}	$+1.6022 \times 10^{-19}$	+1
Neutron	1.67493×10^{-24}	0	0

*More refined measurements have given us a more accurate value of an electron's mass than Millikan's.

mass p ≈ mass n ≈ 1840 x mass e⁻

Atomic number, Mass number and Isotopes

Atomic number (Z) = number of protons in nucleus

Mass number (A) = number of protons + number of neutrons

= atomic number (Z) + number of neutrons

Isotopes are atoms of the same element (X) that have the same atomic number but different mass numbers





The Isotopes of Hydrogen



Isotope	Atomic Number	Number of protons	Number of Neutrons	Number of electrons	mass (amu)
Hydrogen-1	1	1	0	1	1
Hydrogen-2 (deuterium)	1	1	1	1	2
Hydrogen-3 (tritium)	1	1	2	1	3

How many protons, neutrons, and electrons are $in_{6}^{14}C$?

6 protons, 8 (14 - 6) neutrons, 6 electrons

How many protons, neutrons, and electrons are $in_{6}^{11}C$?

6 protons, 5 (11 - 6) neutrons, 6 electrons

Naturally occurring carbon consists of three isotopes, ¹²C, ¹³C, and ¹⁴C. State the number of protons, neutrons, and electrons in each of the following.

	¹² C	¹³ C	¹⁴ C
	6	6	6
Proton	6	6	6
Neutron	6	7	8
Electron	6	6	6
In naturally occurring magnesium, there are three isotopes.

	otop	<u>es o</u>	<u>r ivig</u>
Atomic symbol	$^{24}_{12}$ Mg	²⁵ ₁₂ Mg	²⁶ ₁₂ Mg
Number of protons	12	12	12
Number of electrons	12	12	12
Mass number	24	25	26
Number of neutrons	12	13	14

leaters and Ma





The Modern Periodic Table

1A																	8A
1 H	Alka											13 3A	14 4A	15 5A	16 6A	17 7A	2 H :
3	≦. ∏											5 B	¢	7 N	8 O	9 17	
Ikal	arth	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 	10	11 1B	12 2B	13 Al		15 P	16 S		dob
i Me	M	21 Sc	22 Ti	23 V		25	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	Groc	33 As	34 Se	Halo	le G
etal	etal	39 Y	40 Zr	41 Nb		Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	5n	51 Sb	52 Te	oger	ias
55 C s	:6 I a	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Fb	83 Bi	84 Po	A.t	80 R h
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112	113	114	115	116	(1 7)	118
		(
	Metals			58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
	Metallo	oids		90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Nonmetals

1

18

A *molecule* is an aggregate of two or more atoms in a definite arrangement held together by chemical forces



A diatomic molecule contains only two atoms



A *polyatomic molecule* contains more than two atoms O_3 , H_2O , NH_3 , CH_4

An *ion* is an atom, or group of atoms, that has a net positive or negative charge.

cation – ion with a positive charge If a neutral atom **loses** one or more electrons it becomes a cation.



anion – ion with a negative charge If a neutral atom **gains** one or more electrons it becomes an anion.



17 protons17 electrons



A *monatomic ion* contains only one atom Na⁺, Cl⁻, Ca²⁺, O²⁻, Al³⁺, N³⁻

A *polyatomic ion* contains more than one atom OH⁻, CN⁻, NH₄⁺, CO₃^{2–}, HCO₃⁻, SO₄^{2–}, PO₄^{3–}, NO₃⁻, NO₂⁻

The names of common polyatomic anions

- end in *ate.*
 - NO₃⁻ nitrate PO₄³⁻ phosphate
- with one oxygen less end in *ite*.
 - NO₂⁻ nitrite PO₃³⁻ phosphite
- with hydrogen attached use the prefix *hydrogen* (or *bi*).
 HCO₃⁻ hydrogen carbonate (bicarbonate)
 HSO₃⁻ hydrogen sulfite (bisulfite)

Common Ions Shown on the Periodic Table



How many protons and electrons are in $^{27}_{13}AI^{3+}$?

13 protons, 10 (13 - 3) electrons

How many protons and electrons are in $^{78}_{34}$ Se²⁻?

34 protons, 36 (34 + 2) electrons

ANY QUESTIONS??





Formulas and Models



A *molecular formula* shows the exact number of atoms of each element in the smallest unit of a substance

An *empirical formula* shows the simplest whole-number ratio of the atoms in a substance



ionic compounds consist of a combination of cations and an anions

- The formula is usually the same as the empirical formula
- The sum of the charges on the cation(s) and anion(s) in each formula unit must equal zero

The ionic compound NaCl









The most reactive **metals** (green) and the most reactive **nonmetals** (blue) combine to form ionic compounds.

Formula of Ionic Compounds



Chemical Nomenclature

Ionic Compounds

- Most are binary compounds, some are ternary compounds
- Often a metal + nonmetal
- Anion (nonmetal), add "ide" to element name

BaCl₂ barium chloride
K₂O potassium oxide
Mg(OH)₂ magnesium hydroxide
KNO₃ potassium nitrate

• Transition metal ionic compounds

- indicate charge on metal with Roman numerals



FeCl₂ 2 Cl⁻ -2 so Fe is +2 iron(II) chloride

FeCl₃ 3 Cl^2 -3 so Fe is +3 iron(III) chloride

 Cr_2S_3 3 S⁻² -6 so Cr is +3 (6/2) chromium(III) sulfide

Element	Possible I	ons Name of Ion		
Chromium	Cr ²⁺ Cr ³⁺	chromium(II) chromium(III)		
Copper	Cu ⁺ Cu ²⁺	copper(I) copper(II)		
Gold	Au ⁺ Au ³⁺	gold(I) gold(III)		
Iron	Fe ²⁺ Fe ³⁺	iron(II) iron(III)		
Lead	Pb ²⁺	lead(II)		
	Pb ⁴⁺	lead(IV)		
FeCl ₂	iron(II) chl	oride		
FeCl ₃	iron(III) chloride			
Cu ₂ S	copper(I) sulfide			
CuCl ₂	copper(II) chloride			
SnCl ₂	tin(II) chloride			
PbBr ₄	lead(IV) bromide			

TABLE 2.2The Acc	The "-ide" Nomenclature of Some Common Monatomic Anions According to Their Positions in the Periodic Table					
Group 4A	Group 5A	Group 6A	Group 7A			
C carbide (C ⁴⁻)* Si silicide (Si ⁴⁻)	N nitride (N ³⁻) P phosphide (P ³⁻)	O oxide (O ²⁻) S sulfide (S ²⁻) Se selenide (Se ²⁻) Te telluride (Te ²⁻)	F fluoride (F ⁻) Cl chloride (Cl ⁻) Br bromide (Br ⁻) I iodide (I ⁻)			

*The word "carbide" is also used for the anion C_2^{2-} .

TABLE 2.3Names and Formulas of and Anions	of Some Common Inorganic Cations	
Cation	Anion	
aluminum (Al ³⁺)	bromide (Br ⁻)	
ammonium (NH ⁺ ₄)	carbonate $(CO_3^{2^-})$	
barium (Ba ²⁺)	chlorate (ClO_3^-)	
cadmium (Cd ²⁺)	chloride (Cl ⁻)	
calcium (Ca ²⁺)	chromate (CrO_4^{2-})	
cesium (Cs ⁺)	cyanide (CN ⁻)	
chromium(III) or chromic (Cr ³⁺)	dichromate $(Cr_2O_7^{2-})$	
cobalt(II) or cobaltous (Co ²⁺)	dihydrogen phosphate (H ₂ PO ₄ ⁻)	
copper(I) or cuprous (Cu ⁺)	fluoride (F ⁻)	
copper(II) or cupric (Cu ²⁺)	hydride (H ⁻)	
hydrogen (H ⁺)	hydrogen carbonate or bicarbonate (HCO ₃ ⁻	
iron(II) or ferrous (Fe ²⁺)	hydrogen phosphate (HPO_4^{2-})	
iron(III) or ferric (Fe ³⁺)	hydrogen sulfate or bisulfate (HSO_4^-)	
lead(II) or plumbous (Pb ²⁺)	hydroxide (OH ⁻)	
lithium (Li ⁺)	iodide (I ⁻)	
magnesium (Mg ²⁺)	nitrate (NO ₃ ⁻)	
manganese(II) or manganous (Mn ²⁺)	nitride (N ³⁻)	
mercury(I) or mercurous $(Hg_2^{2+})^*$	nitrite (NO_2^-)	
mercury(II) or mercuric (Hg ²⁺)	oxide $(O^{2^{-}})$	
potassium (K ⁺)	permanganate (MnO ₄ ⁻)	
rubidium (Rb ⁺)	peroxide (O_2^{2-})	
silver (Ag ⁺)	phosphate (PO_4^{3-})	
sodium (Na ⁺)	sulfate (SO_4^{2-})	
strontium (Sr ²⁺)	sulfide (S ²⁻)	
tin(II) or stannous (Sn ²⁺)	sulfite (SO_3^{2-})	
zinc (Zn^{2+})	thiocyanate (SCN ⁻)	

Flowchart for Naming Ionic Compounds						
	Metal (or NH4 ⁺)	Nonmetal				
Q: Does the positive id	netal form one on or more?	Q: Is the nonmetal ion formed from a single atom or a polyatomic ion with oxygen?				
One	More	Single ion	Polyatomic ion			
Group 1A (1)– 3A (13), Zn, Ag, or Cd	Metal in B Groups 3B–12B, Groups 4A (14) or 5A (15)	Monatomic ion such as Cl ⁻ , S ^{2–}	Polyatomic ion such as CO_3^{2-} or SO_4^{2-}			
Use the name of the element or use "ammonium" for the NH ₄ ⁺ ion.	Use the name of the element <i>and</i> a Roman numeral in parentheses for the positive charge of the ion.	Use the root of the name of the element adding <i>ide</i> ending.	Use the name of the polyatomic with an <i>ate</i> or <i>ite</i> ending.			

- Molecular compounds
 - Nonmetals or nonmetals + metalloids
 - Common names
 - H₂O, NH₃, CH₄,
 - Element furthest to the left in a period and closest to the bottom of a group on periodic table is placed first in formula
 - If more than one compound can be formed from the same elements, use prefixes to indicate number of each kind of atom
 - Last element name ends in *ide*

TABLE 2.4

Greek Prefixes Used in Naming Molecular Compounds

Meaning
1
2
3
4
5
6
7
8
9
10

Molecular Compounds

- HI hydrogen iodide
- NF₃ nitrogen trifluoride
- SO₂ sulfur dioxide
- N₂Cl₄ dinitrogen tetrachloride
- NO₂ nitrogen dioxide
- N₂O dinitrogen monoxide



An *acid* can be defined as a substance that yields hydrogen ions (H⁺) when dissolved in water.

For example: HCl gas and HCl in water

•Pure substance, hydrogen chloride HCI

•Dissolved in water (H₃O⁺ and Cl⁻), hydrochloric acid





TABLE 2.5Some Simple Acids

Anion	Corresponding Acid
F ⁻ (fluoride)	HF (hydrofluoric acid)
Cl ⁻ (chloride)	HCl (hydrochloric acid)
Br ⁻ (bromide)	HBr (hydrobromic acid)
I ⁻ (iodide)	HI (hydroiodic acid)
CN ⁻ (cyanide)	HCN (hydrocyanic acid)
S^{2-} (sulfide)	H_2S (hydrosulfuric acid)
	(H2S Hydrogen sulfide)

An *oxoacid* is an acid that contains hydrogen, oxygen, and another element (the central element).

 HNO_{3} HNO_{2} $H_{2}SO_{4}$ $H_{2}SO_{3}$ $H_{2}CO_{3}$ $H_{3}PO_{4}$

nitric acid nitrous acid sulfuric acid sulfurous acid carbonic acid phosphoric acid

Naming Oxoacids and Oxoanions



The rules for naming *oxoanions, anions of oxoacids,* are as follows:

- 1. When all the H ions are removed from the "-ic" acid, the anion's name ends with "-ate."
- 2. When all the H ions are removed from the "-ous" acid, the anion's name ends with "-ite."
- 3. The names of anions in which one or more but not all the hydrogen ions have been removed must indicate the number of H ions present.

For example: Phosphoric acid : H3PO4

- H₂PO₄⁻ dihydrogen phosphate
- HPO₄²⁻ hydrogen phosphate
- PO₄³⁻ phosphate

TABLE 2.6 Names of Oxoacids and Oxoanions That Contain Chlorine

Acid	Anion
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)

A *base* can be defined as a substance that yields hydroxide ions (OH⁻) when dissolved in water.

NaOH sodium hydroxideKOH potassium hydroxideBa(OH)₂ barium hydroxide

Hydrates are compounds that have a specific number of water molecules attached to them.

- $BaCl_2 \cdot 2H_2O$ barium chloride dihydrate
- LiCl•H₂O lithium chloride monohydrate
- MgSO₄•7H₂O magnesium sulfate heptahydrate
- $Sr(NO_3)_2 \cdot 4H_2O$ strontium nitrate tetrahydrate

 $CuSO_4 \bullet 5H_2O \rightarrow$

copper(II) sulfate pentahydrate



TABLE 2.7 Common and Systematic Names of Some Compounds

Formula	Common Name	Systematic Name
H ₂ O	Water	Dihydrogen monoxide
NH ₃	Ammonia	Trihydrogen nitride
CO_2	Dry ice	Solid carbon dioxide
NaCl	Table salt	Sodium chloride
N_2O	Laughing gas	Dinitrogen monoxide
CaCO ₃	Marble, chalk, limestone	Calcium carbonate
CaO	Quicklime	Calcium oxide
Ca(OH) ₂	Slaked lime	Calcium hydroxide
NaHCO ₃	Baking soda	Sodium hydrogen carbonate
$Na_2CO_3 \cdot 10H_2O$	Washing soda	Sodium carbonate decahydrate
$MgSO_4 \cdot 7H_2O$	Epsom salt	Magnesium sulfate heptahydrate
Mg(OH) ₂	Milk of magnesia	Magnesium hydroxide
$CaSO_4 \cdot 2H_2O$	Gypsum	Calcium sulfate dihydrate

ANY QUESTIONS??





Chapter 3 Mass Relationships in Chemical Reactions

3.1 Atomic Lewis Dot Representation: In the 3.2 Molar mass and Avogadro's number 3.3 Molecularmassell electrons) are 3.4 Percent composition of compounds 3.5 Chemical reactions and abemical equations 3.6 Amounts Versaeltaints 9red products most shell electrons) are
3.7 Limiting represented by dots. 3.8 Reaction yiel
Micro World Macro World atoms & molecules grams

Atomic mass is the mass of an atom in atomic mass units (amu)

One **atomic mass unit** is a mass of onetwelfth of the mass of one carbon-12 atom.



By definition: 1 atom ¹²C "weighs" 12 amu

On this scale

 $^{1}H = 1.00794 \text{ amu}$

 $^{16}O = 15.9994$ amu

The *average atomic mass* is the weighted average of all of the naturally occurring isotopes of the element.





Natural lithium is:

7.42% ⁶Li (6.015 amu) 92.58% ⁷Li (7.016 amu)



Average atomic mass of lithium:

$\frac{7.42 \times 6.015 + 92.58 \times 7.016}{100} = 6.941 \text{ amu}$

1 1A																	18 8A
1 H 1.008	2 2A				24 Cr 52.00 -		Atomic n Atomic m	umber nass				13 3A	14 4A	15 5A	16 6A	17 7A	2 He 4.003
3	4								10								
Li	Be								Ne								
6.941	9.012								20.18								
11 Na 22.99	12 Mg 24.31	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 — 8B —	10	11 1B	12 2B	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
39.10	40.08	44.96	47.88	50.94	52.00	54.94	55.85	58.93	58.69	63.55	65.39	69.72	72.59	74.92	78.96	79.90	83.80
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
85.47	87.62	88.91	91.22	92.91	95.94	(98)	101.1	102.9	106.4	107.9	112.4	114.8	118.7	121.8	127.6	126.9	131.3
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
132.9	137.3	138.9	178.5	180.9	183.9	186.2	190.2	192.2	195.1	197.0	200.6	204.4	207.2	209.0	(210)	(210)	(222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (257)	105 Ha (260)	106 Sg (263)	107 Ns (262)	108 Hs (265)	109 Mt (266)	110	111	112						

Metals Metalloids	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
Nonmetals	90 Th 232.0	91 Pa (231)	92 U 238.0	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (256)	102 No (254)	103 Lr (257)

One-Mole Quantities



The *mole (mol)* is the amount of a substance that contains as many elementary entities (atoms, ions or molecules) as there are atoms in exactly 12 grams of ¹²C.

1 mol = N_A = 6.0221367 x 10²³

Avogadro's number (N_A)

<u>1 mole</u>	Number of Atoms	Arradao's						
1 mole C	$= 6.02 \text{ x } 10^{23} \text{ C atoms}$	Nogadro s						
1 mole Na ⁺	$= 6.02 \text{ x } 10^{23} \text{ Na}^+ \text{ ions}$	NUMBER						
1 mole H_2O	= $6.02 \times 10^{23} \text{ H}_2\text{O}$ molecules							
[•] 1 mole of anything = 6.022×10^{23} units of that thing								





Molar mass is the mass of 1 mole of units (atoms/molecules) in grams



1 mol ¹²C atoms = 6.022 x 10²³ atoms

- 1 ¹²C atom = 12.00 amu
- 1 amu = 1.661 x 10⁻²⁴g
- 1 mol ${}^{12}C$ atoms = 12.00 g ${}^{12}C$
- 1 mol lithium atoms = 6.941 g of Li

 $6.02^2\,\times\,10^{23}$ atoms C



1 mol C atoms

For any element

12.01 g C atoms

Molar Mass from Periodic Table



Molar mass is the atomic mass expressed in grams.



1 mol of C contains 6.022 x 10 ²³ C atoms and has a mass of 12.01 g (molar mass)



 \mathcal{M} = molar mass in g/mol $N_{\mathcal{A}}$ = Avogadro's number

Do You Understand Molar Mass?

How many atoms are in 0.551 g of potassium (K) ?

1 mol of K = 39.10 g of K 1 mol of K = 6.022×10^{23} atoms of K

$$0.551 \text{ gK} \times \frac{1 \text{ mol K}}{39.10 \text{ gK}} \times \frac{6.022 \times 10^{23} \text{ atoms K}}{1 \text{ mol K}} =$$

 8.49×10^{21} atoms of K

Molecular mass (or molecular weight) is the sum of the atomic masses (in amu) in a molecule.



For any molecule

molecular mass in amu = molar mass in grams

1 molecule of SO_2 weighs 64.07 amu 1 mole of SO_2 weighs 64.07 g



Number of atoms in 1 molecule Carbon (C) Hydrogen (H) Oxygen (O)







9 mole C

8 mole H 4 mole O

Do You Understand Molecular Mass?

How many H atoms are in 72.5 g of C_3H_8O ?

moles of $C_3H_8O = 72.5 \text{ g} / 60.095 \text{ g/mol} = 1.21 \text{ mol}$

1 mol C₃H₈O molecules contains 8 mol H atoms 1 mol of H atoms is 6.022×10^{23} H atoms

72.5 g C₃H₈O x $\frac{1 \text{ mol } C_3H_8O}{60 \text{ g } C_3H_8O}$ x $\frac{8 \text{ mol H atoms}}{1 \text{ mol } C_3H_8O}$ x $\frac{6.022 \text{ x } 10^{23} \text{ H atoms}}{1 \text{ mol } H \text{ atoms}}$ = 5.82 x 10^{24} H atoms

Steps: 1. Convert grams of C_3H_8O to moles of C_3H_8O .

- 2. Convert moles of C_3H_8O to moles of H atoms.
- 3. Convert moles of H atoms to number of H atoms.

Formula mass is the sum of the atomic masses (in amu) in a formula unit of an ionic compound.

NaCl



- 1Na 22.99 amu
- 1Cl <u>+ 35.45 amu</u> NaCl 58.44 amu

For any ionic compound

formula mass (amu) = molar mass (grams)

1 formula unit of NaCl = 58.44 amu 1 mole of NaCl = 58.44 g of NaCl **Do You Understand Formula Mass?**

What is the formula mass of $Ca_3(PO_4)_2$?

1 formula unit of $Ca_3(PO_4)_2$

- 3 Ca 3 x 40.08 g/mol
- 2 P 2 x 30.97 g/mol
- 8 O <u>+ 8 x 16.00 g</u>/mol 310.18 g/mol

Units of <u>grams per mole</u> are the most practical for chemical calculations!

Percent composition of an element in a compound =

n x molar mass of element molar mass of compound x 100%

n is the number of moles of the element in 1 mole of the compound (assume you have 1 mole!).



$$\%C = \frac{2 \times (12.01 \text{ g})}{46.07 \text{ g}} \times 100\% = 52.14\%$$
$$\%H = \frac{6 \times (1.008 \text{ g})}{46.07 \text{ g}} \times 100\% = 13.13\%$$
$$\%O = \frac{1 \times (16.00 \text{ g})}{46.07 \text{ g}} \times 100\% = 34.73\%$$

52.14% + 13.13% + 34.73% = 100.0%

Percent Composition and Empirical Formulas



To begin, assume for simplicity that you have 100 g of compound!

Percent Composition and Empirical Formulas



A process in which one or more substances is changed into one or more new substances is a *chemical reaction*.

A *chemical equation* uses chemical symbols to show what happens during a chemical reaction.



- atoms are not gained or lost.
- the number of reactant atoms is equal to the number of product atoms.

Symbols used in chemical equations show

- the states of the reactants.
- the states of the products.
- the reaction conditions.



Symbol	Meaning					
+	Separates two or more formulas					
\longrightarrow	Reacts to form products					
Δ	The reactants are heated					
(<i>s</i>)	Solid					
(<i>l</i>)	Liquid					
(g)	Gas					
(aq)	Aqueous					

How to "Read" Chemical Equations

$$2 \text{ Mg} + \text{O}_2 \longrightarrow 2 \text{ MgO}$$

2 atoms Mg + 1 molecule O₂ makes 2 formula units MgO
2 moles Mg + 1 mole O₂ makes 2 moles MgO
48.6 grams Mg + 32.0 grams O₂ makes 80.6 g MgO
IS NOT

2 grams Mg + 1 gram O₂ makes 2 g MgO

 Write the correct formula(s) for the reactants on the left side and the correct formula(s) for the product(s) on the right side of the equation.

Ethane reacts with oxygen to form carbon dioxide and water

 $C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$

 Change the numbers in front of the formulas (*coefficients*) to make the number of atoms of each element the same on both sides of the equation. Do not change the subscripts.

2
$$C_2H_6$$
 NOT C_4H_{12}

3. Start by balancing those elements that appear in only one reactant and one product.



4. Balance those elements that appear in two or more reactants or products.

5. Check to make sure that you have the same number of each type of atom on both sides of the equation.

 $2 C_2 H_6 + 7 O_2 \longrightarrow 4 CO_2 + 6 H_2 O$ $4 C (2 \times 2) \qquad 4 C$ $12 H (2 \times 6) \qquad 12 H (6 \times 2)$ $14 O (7 \times 2) \qquad 14 O (4 \times 2 + 6)$

Reactants	Products
4 C	4 C
12 H	12 H
14 O	14 O

Acetylene gas C_2H_2 burns in the oxyacetylene torch for welding. How many grams of C_2H_2 are burned if the reaction produces 75.0 g CO₂?

2 $C_2H_2(g) + 5O_2(g) \rightarrow 4 CO_2(g) + 2H_2O(g)$



 $= 22.2 \text{ g } \text{C}_2 \text{H}_2$

Stoichiometry – Quantitative study of reactants and products in a chemical reaction



- 1. Write the **balanced chemical equation**.
- 2. Convert quantities of known substances into moles.
- 3. Use **coefficients** in balanced equation to calculate the number of **moles of the sought quantity**.
- 4. Convert moles of sought quantity into the desired units.

Methanol burns in air according to the equation

 $2 \text{ CH}_3\text{OH} + 3 \text{ O}_2 \longrightarrow 2 \text{ CO}_2 + 4 \text{ H}_2\text{O}$

If 209 g of methanol are used up in the combustion, what mass of water is produced?

grams $CH_3OH \longrightarrow moles CH_3OH \longrightarrow moles H_2O \longrightarrow grams H_2O$

$$209 \text{ g CH}_{3}\text{OH} \times \frac{1 \text{ mol CH}_{3}\text{OH}}{32.0 \text{ g CH}_{3}\text{OH}} \times \frac{4 \text{ mol H}_{2}\text{O}}{2 \text{ mol CH}_{3}\text{OH}} \times \frac{18.0 \text{ g H}_{2}\text{O}}{1 \text{ mol H}_{2}\text{O}} =$$

235 g of H_2O

Limiting reagent – the reactant used up first in a reaction, controlling the amounts of products formed

Excess reagents – the reactants present in quantities greater than necessary to react with the quantity of the limiting regent

Limiting Reactant

5 cars + 200 drivers \longrightarrow Limiting cars or drivers? 50 chairs + 15 students \longrightarrow Limiting chairs or students?



Determining the Limiting Reactant

(the one gives the least amount of product)

If you heat 2.50 mol of Fe and 3.00 mol of S, how many moles of FeS are formed?

 $Fe(s) + S(s) \rightarrow FeS(s)$

- According to the balanced equation, 1 mol of Fe reacts with 1 mol of S to give 1 mol of FeS.
- So 2.50 mol of Fe will react with 2.50 mol of S to produce 2.50 mol of FeS.
- Therefore, iron is the limiting reactant and sulfur is the excess reactant.

Mass Limiting Reactant Problems

There are three steps to a limiting reactant problem:

1. Calculate the mass of product that can be produced from the first reactant.

mass reactant #1 \Rightarrow mol reactant #1 \Rightarrow mol product \Rightarrow mass product

2. Calculate the mass of product that can be produced from the second reactant.

mass reactant $#2 \Rightarrow$ mol reactant $#2 \Rightarrow$ mol product \Rightarrow mass product

3. The limiting reactant is the reactant that produces the <u>least</u> amount of product.

In a reaction, 124 g of AI are reacted with 601 g of Fe_2O_3 .

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

Calculate the mass of Al_2O_3 formed in grams.

- 1. Balanced reaction: Done.
- 2. Moles of "given" reactants. Moles of AI = 124 g / 26.9815 g/mol = 4.60 mol Moles of Fe₂O₃ = 601 g / 159.6882 g/mol = 3.76 mol
- 3. Moles of "desired" product, Al_2O_3 .

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

Moles of $Al_2O_3 = 3.76 \text{ mol Fe}_2O_3 \times 1 \text{ mol } Al_2O_3 = 3.76 \text{ mole } Al_2O_3$ based on Fe $_2O_3 = 1 \text{ mol Fe}_2O_3$ **Keep the smaller answer!** All is the limiting reactant. **4.** Grams of $Al_2O_3 = 2.30 \text{ mol } \times 101.9612 \text{ g/mol} = 235 \text{ g}$ How many grams of AgBr can be formed when solutions containing 50 g MgBr₂ and 100 g AgNO₃ are mixed together ? how many grams of the excess reactant remain unreacted?

 $MgBr_2 + 2AgNO_3 \longrightarrow 2AgBr + Mg(NO_3)_2$

mole ratio: 1 mol MgBr₂ \iff 2 mol AgNO₃ \iff 2 mol AgBr

- $(50/184.1) \text{ mol MgBr}_2 \quad X \quad \underline{2 \text{ mol AgBr}}_2 \quad X \quad 187.8 = 102 \text{ g AgBr}$ 1 mol MgBr_2
- $(100/169.9) \text{ mol AgNO}_3 \times 2 \text{ mol AgBr} \times 187.8 = 110.5 \text{ g AgBr}$ 2 mol AgNO₃
 - $MgBr_2 = limiting reactant \implies 102 g AgBr is yielded$
 - $(50/184.1) \text{ mol MgBr}_2 \quad \chi \quad \underline{2 \text{ mol AgNO}_3} \quad \chi \quad 169.9. = 92.3 \text{gAgNO}_3 \\ 1 \text{ mol MgBr}_2$

100 -92.3 = 7.7 g AgNO₃ unreacted

Reaction Yield

Theoretical Yield is the amount of product that would result if all the limiting reagent reacted. Can be obtained from calculation based on balanced equation.

Actual Yield is the amount of product actually obtained from a reaction. Can be obtained from the given problem.

Percent yield is the amount of the actual yield compared to the theoretical yield.

% Yield = $\frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$

Suppose a student performs a reaction and obtains
 0.875 g of CuCO₃ and the theoretical yield is
 0.988 g. What is the percent yield?

 $\operatorname{Cu}(\operatorname{NO}_3)_2(aq) + \operatorname{Na}_2\operatorname{CO}_3(aq) \rightarrow \operatorname{Cu}\operatorname{CO}_3(s) + 2\operatorname{Na}\operatorname{NO}_3(aq)$

$$\frac{0.875 \text{ g } \text{CuCO}_3}{0.988 \text{ g } \text{CuCO}_3} \times 100 \% = 88.6 \%$$

• The percent yield obtained is 88.6%.

ANY QUESTIONS??




Reactions in Aqueous Solution Chapter 4

4.1 General Properties of Aqueous Solutions
4.2 Precipitation Reactions
4.3 Acid- Base Reactions
4.4 Oxidation – Reduction Reactions
4.4 Concentration of Solutions
4.5 Titration



sodium (Na) chlorine (CI)





4.1 General Properties of Aqueous Solutions

A *solution* is a homogenous mixture of 2 or more substances





Sea water Vinegar H₂O H₂O

Salt (NaCl) Acetic acid

 (CH_3COOH)

Туре	Example	Solute	Solvent
Gas Solutions			
Gas in a gas	Air	Oxygen (gas)	Nitrogen (gas)
Liquid Solutions			
Gas in a liquid	Soda water	Carbon dioxide (gas)	Water (liquid)
	Household ammonia	Ammonia (gas)	Water (liquid)
Liquid in a liquid	Vinegar	Acetic acid (liquid)	Water (liquid)
Solid in a liquid	Seawater	Sodium chloride (solid)	Water (liquid)
(liquid)	Tincture of iodine	Iodine (solid)	Alcohol
Solid Solutions			
Liquid in a solid	Dental amalgam	Mercury (liquid)	Silver (solid)
Solid in a solid	Brass	Zinc (solid)	Copper (solid)
	Steel	Carbon (solid)	Iron (solid)

Identify the solute in each of the following solutions.

- A. 2 g sugar and 100 mL water
- B. 60.0 mL of ethyl alcohol and 30.0 mL of methyl alcohol
- C. 55.0 mL water and 1.50 g NaCl
- D. Air: 200 mL O_2 and 800 mL N_2

Two types of Solutes

Non-electrolyte

When dissolved in water does not conduct electricity



When dissolved in water can conduct electricity



Non-electrolyte



weak electrolyte



strong electrolyte

Electrolyte conduct electricity in solution? Dissociation= The splitting of a molecule into smaller molecules, atoms, or ions Ionization= Separation of atom/molecules into ions

Strong Electrolyte –Complete (100%) dissociation

NaCl (s)
$$\xrightarrow{H_2O}$$
 Na⁺ (aq) + Cl⁻ (aq)

Non-reversible reaction



Weak Electrolyte – Incomplete (<100%) dissociation

$$HF(g) \longrightarrow H^+(aq) + F^-(aq)$$

 $CH_3COOH \implies CH_3COO^-(aq) + H^+(aq)$

Reversible reaction



Non-electrolyte does not conduct electricity?

$$C_6H_{12}O_6(s) \xrightarrow{2} C_6H_{12}O_6(aq)$$

No cations (+) and anions (-)
in solution. Exist in solution as

H₂O

neutral molecules.





Nonelectrolyte



Weak electrolyte

ABLE 4.1	Classification	of Solutes	in Aa	ueous	Solution
	classification	01 3010103	III AY	00003	301011011

STRONG ELECTROLYTE	WEAK ELECTROLYTE	NONELECTROLYTE
HCl	CH ₃ COOH	(NH ₂) ₂ CO (urea)
HNO ₃	HF	CH ₃ OH (methanol)
HClO ₄	HNO ₂	C ₂ H ₅ OH (ethanol)
$H_2SO_4^*$	NH ₃	C ₆ H ₁₂ O ₆ (glucose)
NaOH	$\rm H_2O^\dagger$	C ₁₂ H ₂₂ O ₁₁ (sucrose)
Ba(OH) ₂		
Ionic compounds		

Pure water contains very few ions, cannot conduct electricity (extremely weak electrolyte)

Water

- electrically neutral molecule
- positive and negative region (pole)
- polar solvent (for ionic compounds)

Hydration



 the process in which an ion is surrounded by water molecules arranged in a specific manner.

• helps to stabilize ions in solution and prevents cations from combining with anions. Partial negative



When NaCI dissolves in water,Na⁺ ions and Cl⁻ ions are separated from each other and undergo "hydration".



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4.2 Precipitation Reactions

Precipitation= Reaction that results in the formation of an insoluble product (precipitate)

Precipitate= insoluble solid that separates from solution

Metathesis/ double-displacement reaction

= reaction that involves the exchange of parts

between two compounds

Example: Precipitation of Lead Iodide



Molecular equation (species as molecule)

 $Pb(NO_3)_2(aq) + 2Nal(aq) \longrightarrow Pbl_2(s) + 2NaNO_3(aq)$

Ionic equation (species as dissolved free ions) $Pb^{2+}(aq) + 2NO_3(aq) + 2Na^+(aq) + 2I^-(aq)$ $\longrightarrow PbI_2(s) + 2Na^+(aq) + 2NO_3(aq)$

Na⁺ and NO₃⁻ are *spectator* ions (does not involved in the overall reaction)

Net ionic equation (species that actually take part in the reaction)

 $Pb^{2+}(aq) + 2l^{-}(aq) \longrightarrow Pbl_{2}(s)$



Pbl₂



Writing Net Ionic Equations

- 1. Write the balanced molecular equation.
- 2. Write the ionic equation showing the strong electrolytes completely dissociated into cations and anions.
- 3. Cancel the spectator ions on both sides of the ionic equation
- 4. Check that charges and number of atoms are balanced in the net ionic equation

Write the net ionic equation for the reaction of silver nitrate with sodium chloride.

$$AgNO_3(aq) + NaCI(aq) \longrightarrow AgCI(s) + NaNO_3(aq)$$

 $Ag^{+}(aq) + NO_{3}^{-}(aq) + Na^{+}(aq) + CI^{-}(aq)$ $\longrightarrow AgCI(s) + Na^{+}(aq) + NO_{3}^{-}(aq)$

$$Ag^{+}(aq) + CI^{-}(aq) \longrightarrow AgCI(s)$$

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Solubility= Maximum amount of solute that will dissolve in a given quantity of solvent in a specific temperature.

Substances > Soluble/ slightly soluble/ insoluble

Solubility rules – to predict the solubility of ionic compounds

TABLE 4.2 Solubility Rules for Common Ionic Compounds in Water at 25°C

Soluble Compounds	Insoluble Exceptions					
Compounds containing alkali metal ions (Li^+ , Na^+ , K^+ , Rb^+ , Cs^+) and the ammonium ion (NH_4^+)						
Nitrates (NO_3^-) , bicarbonates (HCO_3^-) , and chlorates (ClO_3^-)						
Halides (Cl ⁻ , Br ⁻ , I ⁻)	Halides of Ag^+ , Hg_2^{2+} , and Pb^{2+}					
Sulfates (SO_4^{2-})	Sulfates of Ag^+ , Ca^{2+} , Sr^{2+} , Ba^{2+} , Hg_2^{2+} , and Pb^{2+}					
Insoluble Compounds	Soluble Exceptions					
Carbonates $(CO_3^{2^-})$, phosphates $(PO_4^{3^-})$, chromates $(CrO_4^{2^-})$, sulfides (S^{2^-})	Compounds containing alkali metal ions and the ammonium ion					
Hydroxides (OH ⁻)	Compounds containing alkali metal ions					

and the Ba^{2+} ion



4.3 Acid- Base Reactions

Properties of Acids

- Substance that ionize in water to produce H + ions (Arrhenius)
- •Have a sour taste, eg. vinegar (acetic acid), citrus fruits (citric acid).
- Change litmus (plant dyes) from blue to red.
- React with metals (Zn, Mg, Fe) to produce H₂.

 $2\text{HCl}(aq) + \text{Mg}(s) \longrightarrow \text{MgCl}_2(aq) + \text{H}_2(g)$

React with carbonates/bicarbonates to produce CO₂

 $2\text{HCl}(aq) + \text{Na}_2\text{CO}_3(aq) \longrightarrow 2\text{NaCl}(aq) + \text{CO}_2(g) + \text{H}_2\text{O}(l)$

• Aqueous acid solutions conduct electricity.





Properties of Bases

- Substance that ionize in water to produce OH- ion (Arrhenius)
- Have a bitter taste.
- Feel slippery. Many soaps contain bases.
- Change litmus from red to blue
- Aqueous base solutions conduct electricity.





Arrhenius acid is a substance that produces $H^+(H_3O^+)$ in water



Arrhenius base is a substance that produces OH⁻ in water



A *Brønsted acid* is a proton donor A *Brønsted base* is a proton acceptor

HCI is Bronsted acid because it donates proton

 $HCl(aq) \longrightarrow H^{+}(aq) + Cl^{-}(aq)$ $HCl(aq) + H_{2}O(l) \longrightarrow H_{3}O^{+}(aq) + Cl^{-}(aq)$

H₃O⁺ = Hydrated proton (Hydronium)

NH₃ is Bronsted base because it accepts proton

$$NH_{3}(aq) + H^{+}(aq) \implies NH_{4}^{+}(aq)$$
$$NH_{3}(aq) + H_{2}O(l) \implies NH_{4}^{+}(aq) + OH^{-}(aq)$$

TABLE 4.3

Some Common Strong and Weak Acids

Strong Acids	Weak Acids						
Hydrochloric acid	HC1	Hyd acid	rofluoric	HF			
Hydrobromic acid Hydroiodic	HBr HI	Nitro Phos	ous acid sphoric acid	HNO ₂ H ₃ PO ₄			
acid	111	Ace	tic acid	CH ₃ COOH			
Nitric acid	HNO_3						
Sulfuric acid	H_2SO_4						
Perchloric acid	$HClO_4$			22			

Identify each of the following species as a Brønsted acid, base, or both.

(a) HI, (b) CH_3COO^- , (c) $H_2PO_4^-$

 $HI(aq) \longrightarrow H^+(aq) + I^-(aq)$ Brønsted acid

 $CH_3COO^-(aq) + H^+(aq) \implies CH_3COOH(aq)$ Brønsted base

 $H_2PO_4^-(aq) \Longrightarrow H^+(aq) + HPO_4^{2-}(aq)$ Brønsted acid

 $H_2PO_4^-(aq) + H^+(aq) \rightleftharpoons H_3PO_4(aq)$ Brønsted base

Amphoteric = having both acid and basic properties.

Neutralization Reaction

A reaction between an acid and a base, results in a salt and water .

 $acid + base \longrightarrow salt + water$

 $HCI (aq) + NaOH (aq) \longrightarrow NaCI (aq) + H_2O(I)$

 $\begin{array}{r} \mathsf{H}^+(aq) + \mathsf{CI}^+(aq) + \mathsf{Na}^+(aq) + \mathsf{OH}^+(aq) \\ & \longrightarrow & \mathsf{Na}^+(aq) + \mathsf{CI}^+(aq) + \mathsf{H}_2\mathsf{O}(l) \\ \end{array}$

 $H^{+}(aq) + OH^{-}(aq) \longrightarrow H_{2}O(l)$

4.4 Oxidation-Reduction / Redox Reactions



Oxidation-Reduction/ Redox Reactions

(electron transfer reactions)

Example: formation of MgO from Mg and O₂

Oxidation reaction:
half-reaction involves lose e⁻Reduction reaction:
half-reaction involves gain e⁻
 $O_2 + 4e^- \longrightarrow 2O^{2-}$

Half reaction: Reaction that shows e- involved in redox reaction



 $Zn (s) + CuSO_4 (aq) \longrightarrow ZnSO_4 (aq) + Cu (s)$ $Zn \longrightarrow Zn^{2+} + 2e^{-}$ Zn is oxidized Zn is the *reducing agent* $Cu^{2+} + 2e^{-} \longrightarrow Cu$ Cu^{2+} is reduced Cu^{2+} is the *oxidizing agent*

> Copper wire reacts with silver nitrate to form silver metal. What is the oxidizing agent in the reaction?

Cu (s) + 2AgNO₃ (aq) \longrightarrow Cu(NO₃)₂ (aq) + 2Ag (s)Cu \longrightarrow Cu²⁺ + 2e⁻ Cu is oxidized Ag⁺ is reduced Cu is the *reducing agent* Ag⁺ is the **oxidizing agent**



Oxidation number

The charge the atom would have in a molecule (or an ionic compound) if electrons were completely transferred.

1. Free elements (uncombined state) have an oxidation number of zero.

Na, Be, K, Pb,
$$H_2$$
, O_2 , $P_4 = 0$

2. In monatomic ions, the oxidation number is equal to the charge on the ion.

3. The oxidation number of oxygen is **usually** –2. In H_2O_2 and $O_2^{2^-}$ it is –1.



- 4. The oxidation number of hydrogen is +1 *except* when it is bonded to metals in binary compounds (eg. LiH, NaH, CaH₂). In these cases, its oxidation number is -1
- Group IA metals are +1, IIA metals are +2 and fluorine is always -1.
 - 6. The sum of the oxidation numbers of all the atoms in a neutral molecule is equal to 0. The sum of oxidation numbers of all the element in polyatomic ion is equal to the charge of the ion.
- 7. Oxidation numbers do not have to be integers. Oxidation number of oxygen in the superoxide ion, O_2^- , is $-\frac{1}{2}$.

What are the oxidation numbers of the element in the following ?

$$HCO_3^-$$
 IF₇ NalO₃ K₂Cr₂O₇

The Oxidation Numbers of Elements in their Compounds

1 1A H +1 -1		•	Me [:] Noi Ele	tallio n-m mer	c ele etall nts i	eme lic e n gr	nt: - Iem oup	+ve ents 1A	oxic 8: +\ -7A	datic /e/-\ can	on n /e o ha\	umt xida /e o	oers ation xida	nu nu	mbe 1	ers	18 8A 2 He
	2 2A		nur	nbe	rs=(grou	ip ni	umk	ber			13 3A	14 4A	15 5A	16 6A	17 7A	
3 Li +1	4 Be +2	•	Tra po:	nsit ssib	ion le o	met xida	als I Ition	have nu	e ma mbe	any ers		5 B +3	6 C +4 +2 -4	7 N +5 +4 +3 +2 +1 -3	8 +2 $-\frac{1}{-2}$ -1 -2	9 F -1	10 Ne
11 Na +1	12 Mg +2	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 —8B—	10	11 1B	12 2B	13 Al +3	14 Si +4 -4	15 P +5 +3 -3	16 S +6 +4 +2 -2	17 Cl +7 +65 +43 +1 -1	18 Ar
19 K +1	20 Ca +2	21 Sc +3	22 Ti +4 +3 +2	23 V +5 +4 +3 +2	24 Cr +6 +5 +4 +3 +2	25 Mn +7 +6 +4 +3 +2	26 Fe +3 +2	27 Co +3 +2	28 Ni +2	29 Cu +2 +1	30 Zn +2	31 Ga +3	32 Ge +4 -4	33 As +5 +3 -3	34 Se +6 +4 -2	35 Br +5 +3 +1 -1	36 Kr +4 +2
37 Rb +1	38 Sr +2	39 Y +3	40 Zr +4	41 Nb +5 +4	42 Mo +6 +4 +3	43 Tc +7 +6 +4	44 Ru +8 +6 +4 +3	45 Rh +4 +3 +2	46 Pd +4 +2	47 Ag +1	48 Cd +2	49 In +3	50 Sn +4 +2	51 Sb +5 +3 -3	52 Te +6 +4 -2	53 I +7 +5 +1 -1	54 Xe +6 +4 +2
55 Cs +1	56 Ba +2	57 La +3	72 Hf +4	73 Ta +5	74 W +6 +4	75 Re +7 +6	76 Os +8 +4	77 Ir +4 +3	78 Pt +4 +2	79 Au +3 +1	80 Hg +2 +1	81 Tl +3 +1	82 Pb +4 +2	83 Bi +5 +3	84 Po +2	85 At -1	86 Rn

Redox reaction can be explained in term of

Oxidation	Aspect	Reduction
Loss of electrons	Gain/loss of electron	Gain electrons
Increase in oxidation number	Increase/decrease in oxidation number	Decrease in oxidation number

Types of Oxidation-Reduction Reactions

- 1. Combination reaction
- 2. Decomposition reaction
- 3. Combustion reaction
- 4. Displacement reaction
- 5. Disproportionation reaction

Combination Reaction

Two or more substances combine to form a single product.

 $A + B \longrightarrow C$

$$2AI + 3Br_2 \longrightarrow 2AIBr_3$$

Decomposition Reaction

Breakdown of a compound into two or more components.





 $C \longrightarrow A + B$ $\stackrel{+1+5-2}{2\text{KCIO}_3} \longrightarrow \stackrel{+1-1}{2\text{KCI}} \stackrel{0}{\xrightarrow{}}_2$



Combustion Reaction

Reaction of a substance with oxygen, usually with the release

of heat and light to produce a flame







$${}^{0}_{2} \overset{0}{\longrightarrow} {}^{+2}_{2} \overset{-2}{\longrightarrow} 2MgO$$



Displacement Reaction

An ion/atom in a compound is replaced by an ion/atom of another element

 $A + BC \longrightarrow AC + B$

- 1.Hydrogen Displacement
- 2. Metal Displacement
- 3. Halogen Displacement


1.Hydrogen Displacement

Displace of H (from water or acid) by metal



 $\overset{0}{Z}n + \overset{+1}{2}HCI \longrightarrow \overset{+2}{Z}nCI_2 + \overset{0}{H_2}$

2. Metal Displacement

Displace of metal by another metal

The Activity Series for Metals

(the strength as reducing agent) $2K + 2H_2O \longrightarrow 2KOH + H_2$ (fast) strengt $Mg + 2H_2O \longrightarrow Mg(OH)_2 + H_2(slow)$ $Cu + 2H_2O \longrightarrow$ no reaction Reactivity K > Mg > Cu

 $Li \rightarrow Li^+ + e^ K \rightarrow K^+ + e^ Ba \rightarrow Ba^{2+} + 2e^{-}$ $Ca \rightarrow Ca^{2+} + 2e^{-}$ $Na \rightarrow Na^+ + e^ Mg \rightarrow Mg^{2+} + 2e^{-}$ $Al \rightarrow Al^{3+} + 3e^{-}$ $Zn \rightarrow Zn^{2+} + 2e^{-}$ React with steam $Cr \rightarrow Cr^{3+} + 3e^{-}$ to produce H_2 $Fe \rightarrow Fe^{2+} + 2e^{-}$ $Cd \rightarrow Cd^{2+} + 2e^{-}$ $C_0 \rightarrow C_0^{2+} + 2e^{-}$ $Ni \rightarrow Ni^{2+} + 2e^{-}$ $\operatorname{Sn} \rightarrow \operatorname{Sn}^{2+} + 2e^{-}$ $Pb \rightarrow Pb^{2+} + 2e^{-}$ $H_2 \rightarrow 2H^+ + 2e^ Cu \rightarrow Cu^{2+} + 2e^{-}$ $Ag \rightarrow Ag^+ + e^ Hg \rightarrow Hg^{2+} + 2e^{-}$ $Pt \rightarrow Pt^{2+} + 2e^{-}$ $Au \rightarrow Au^{3+} + 3e^{-}$

React with cold water to produce H_2

React with acids to produce H_2

Do not react with water or acids to produce H₂

3. Halogen Displacement Reaction

Displace of halogen by another halogen

The Activity Series for Halogens (the strength as oxidizing agent)

$$F_2 > CI_2 > Br_2 > I_2$$

$$\overset{0}{\text{Cl}_{2}} + 2 \overset{-1}{\text{KBr}} \longrightarrow 2 \overset{-1}{\text{KCl}} + \overset{0}{\text{Br}_{2}}$$

$$\overset{0}{\text{Cl}_{2}} + 2 \overset{-1}{\text{Nal}} \longrightarrow 2 \overset{-1}{\text{NaCl}} + \overset{0}{\text{I}_{2}}$$

$$\overset{1}{\text{I}_{2}} + \overset{1}{\text{KBr}} \longrightarrow \text{ no reaction}$$

4. Disproportionation Reaction

The same element is simultaneously oxidized and reduced.



Classify each of the following reactions. Precipitation $Ca^{2+} + CO_3^{2-} \longrightarrow CaCO_3$ Metathesis/ $BaCl_2 + NaSO_4 \longrightarrow NaCl_2 + BaSO_4$ Double displacement $Zn + 2HCI \longrightarrow ZnCI_2 + H_2$ Redox (H₂ Displacement) $Ca + F_2 \longrightarrow CaF_2$ Redox (Combination) $2H_2O \longrightarrow O_2 + 2H_2$ Redox (decomposition) $2H_2O_2 \rightarrow 2H_2O + O_2$ Redox (disproportionation) -2 0 -1

4.4 Concentration of Solutions





Concentration= amount of solute in a given quantity of solution.

Molarity/ molar concentration (M)

- The number of moles of solute in 1 liter (L) of solution
- Unit= moles/liter (mol/L)

moles o	of solute	(mol)

liters of solution (L)

$$M = \frac{n}{V}$$

moles = molarity (mol/L) × volume (L)

= MV

M = molarity =



Dilution is the procedure for preparing a less concentrated solution from a more concentrated solution.



What mass of KI is required to make 500mL of a 2.80 *M* KI solution?

volume of KI solution $\xrightarrow{M \text{ KI}}$ moles KI $\xrightarrow{M \text{ KI}}$ grams KI 500. mL x $\frac{1 \text{ L}}{1000 \text{ pL}}$ x $\frac{2.80 \text{ mol KI}}{1 \text{ L soln}}$ x $\frac{166 \text{ g KI}}{1 \text{ mol KI}}$ = 232 g KI How would you prepare 60.0 mL of 0.200 M HNO₃ from a stock solution of 4.00 M HNO₃?

$$M_i V_i = M_f V_f$$

$$M_{\rm i} = 4.00 \ M \ M_{\rm f} = 0.200 \ M \ V_{\rm f} = 0.0600 \ L \ V_{\rm i} = ? \ L$$

 $V_{i} = \frac{M_{f}V_{f}}{M_{i}} = \frac{0.200 \ M \times 0.0600 \ L}{4.00 \ M} = 0.00300 \ L = 3.00 \ mL$

Dilute 3.00 mL of HNO_3 with water to a total volume of 60.0 mL.



4.5 Titration





Titrations -A solution of **known concentration** (standard solution) is added gradually to another solution of **unknown concentration** until the **chemical reaction** between the two solutions is **complete**.

Equivalence point – the point at which the reaction is complete

- *End point* the point at which the indicator permanently changes its color
- *Indicator* substance that changes color at (or near) the equivalence point (eg. phenolphthalein)
- Slowly add standardized base to unknown acid until the indicator changes color



Titrations can be used in the analysis of

Acid-base reactions (transfer of H⁺)

- $H_2SO_4 + 2NaOH \longrightarrow 2H_2O + Na_2SO_4$
- $2H^+$ + $2OH^- \longrightarrow 2H_2O$

Redox reactions (transfer of e⁻)

- 10 $FeSO_4 + 2 KMnO_4 + 8 H_2SO_4 \longrightarrow 5 Fe_2(SO_4)_3 + 2 MnSO_4 + K_2SO_4 + 8 H_2O$
- $5Fe^{2+} + MnO_4^{-} + 8H^+ \longrightarrow 5Fe^{3+} + Mn^{2+} + 4H_2O$



What volume of a 1.420 M NaOH solution is required to titrate 25.00 mL of a 4.50 M H₂SO₄ solution?



16.42 mL of 0.1327 MKMnO₄ solution is needed to oxidize 25.00 mL of an acidic FeSO₄ solution. What is the molarity of the iron solution?





Chapter 5 Gases

5.1 SUBSTANCES THAT EXIST AS GASES 5.2 PRESSURE OF A GAS 5.3 THE GAS LAWS 5.4 THE IDEAL GAS EQUATION 5.5 GAS STOICHIOMETRY 5.6 DALTON'S LAW OF PARTIAL PRESSURES 5.7 THE KINETIC MOLECULAR THEORY OF GASES 5.8 DEVIATION FROM IDEAL BEHAVIOR

5.1 Substances that exist as

gases



Elemental state at 25°C and 1 atmosphere



Physical Characteristics of Gases

- Take the volume and shape of their containers
- Most compressible
- Mix evenly and completely when confined to the same container
- Low Densities

Property	Solid	Liquid	Gas
Density	High	High (like solids)	Low
Shape	Fixed	Takes shape of low part of container	Expands to fill the container
Compressibility	Small	Small	Large

TABLE 5.1 Some Substances Found as Gases at 1 atm and 25°C

Elements	Compounds
H ₂ (molecular hydrogen)	HF (hydrogen fluoride)
N ₂ (molecular nitrogen)	HCl (hydrogen chloride)
O ₂ (molecular oxygen)	HBr (hydrogen bromide)
O ₃ (ozone)	HI (hydrogen iodide)
F ₂ (molecular fluorine)	CO (carbon monoxide)
Cl ₂ (molecular chlorine)	CO ₂ (carbon dioxide)
He (helium)	NH ₃ (ammonia)
Ne (neon)	NO (nitric oxide)
Ar (argon)	NO ₂ (nitrogen dioxide)
Kr (krypton)	N ₂ O (nitrous oxide)
Xe (xenon)	SO ₂ (sulfur dioxide)
Rn (radon)	H ₂ S (hydrogen sulfide)
	HCN (hydrogen cyanide)*

*The boiling point of HCN is 26°C, but it is close enough to qualify as a gas at ordinary atmospheric conditions.

5.2 Pressure of a gas





1 pascal (Pa) = 1 N/m^2

Standard atmospheric pressure (1 atm)

- = the pressure that support a column of mercury exactly 760mmHg high at 0 °C at sea level
- = 760 mmHg
- = 760 torr
- = 101,325 Pa
- = 101.325 KPa

1 pascal (Pa) = 1 N/m^2

1 atm = 760 mmHg = 760 torr = 101,325 Pa

Barometer

A barometer

- measures the pressure exerted by the gases in the atmosphere.
- indicates atmospheric pressure as the height in mm of the mercury column.



A. What is 475 mm Hg expressed in atm?

$$\begin{array}{rcl} 475 \text{ mm Hg} & \text{x} & \underline{1 \text{ atm}} & = & 0.625 \text{ atm} \\ & & 760 \text{ mm Hg} \end{array}$$

B. The pressure of a tire is measured as 2.00 atm. What is this pressure in mm Hg?

 $2.00 \text{ atm } x \frac{760 \text{ mm Hg}}{1 \text{ atm}} = 1520 \text{ mm Hg}$



Atmospheric pressure

= pressure exerted by earth's atmosphere. eg drink liquid through a straw

Properties That Describe a Gas

Gases are described in terms of four properties:

pressure (P), volume(V), temperature(T), and amount(n).

Property	Description	Unit(s) of Measurement
Pressure (P)	The force exerted by gas against the walls of the container	atmosphere (atm); mm Hg; torr; pascal
Volume (V)	The space occupied by the gas	liter (L); milliliter (mL)
Temperature (T)	Determines the kinetic energy and rate of motion of the gas particles	Celsius (°C); Kelvin (K) required in calculations
Amount (n)	The quantity of gas present in a container	grams (g); moles (n) required in calculations

- There are three variables that affect gas *pressure*:
 - 1) The *volume* of the container.
 - 2) The *temperature* of the gas.
 - 3) The *<u>number of molecules</u>* of gas in the container.

5.3 The Gas Laws



The Gas Law

The relationship between **volume**, **pressure**, **temperature** and **moles**

Boyle' s Law Charles's Law Avogadro's Law

The **Ideal Gas Equation** combines several of these laws into a single relationship.

Boyle's Law

The volume of a fixed amount of gas at constant temperature is inversely proportional to the gas pressure



Boyle's Law



• if volume decreases, the pressure increases.

A sample of chlorine gas occupies a volume of 946 mL at a pressure of 726 mmHg. What is the pressure of the gas (in mmHg) if the volume is reduced at constant temperature to 154 mL?

$$P \times V = constant$$

 $P_1 \times V_1 = P_2 \times V_2$
 $P_1 = 726 \text{ mmHg}$ $P_2 = ?$
 $V_1 = 946 \text{ mL}$ $V_2 = 154 \text{ mL}$

$$P_2 = \frac{P_1 \times V_1}{V_2} = \frac{726 \text{ mmHg x 946 mL}}{154 \text{ mL}} = 4460 \text{ mmHg}$$

Charles' & Gay-Lussac's Law



Charles' Law

the volume of a fixed amount of gas at constant pressure is *directly proportional* to the absolute temperature (in Kelvin) of the gas



Charles' Law



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If temperature of a gas increases, its volume increases.

- Below is an illustration of Charles's law.
- As a balloon is cooled from room temperature with liquid nitrogen (-196 °C), the volume decreases.


A balloon has a volume of 785 mL at 21°C. If the temperature drop to 0°C, what is the new volume of the balloon (P constant)?

$$\frac{V_{1}}{T_{1}} = \frac{V_{2}}{T_{2}}$$

$$V_{2} = \frac{V_{1}}{T_{1}} \times \frac{T_{2}}{T_{1}}$$

$$= 785 \text{ mL} \times \frac{(0+273.15) \text{ K}}{(21+273.15) \text{ K}} = 729 \text{ mL}$$

Avogadro's Law

At constant pressure and temperature, volume of gas is directly proportional to the number of moles of the gas

 $V\alpha$ number of moles (*n*)

V = k n T and P are constant $\frac{V}{n} = k$ $\frac{V_1}{n} = \frac{V_2}{n_2}$



If the number of moles (*n*) of gas increase, the volume increase

Avogadro's Law



Ammonia burns in oxygen to form nitric oxide (NO) and water vapor. How many volumes of NO are obtained from one volume of ammonia at the same temperature and pressure?

 $4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$ 1 mole $NH_3 \longrightarrow 1$ mole NOAt constant T and P1 volume $NH_3 \longrightarrow 1$ volume NO If 0.75 mole helium gas occupies a volume of 1.5 L, what volume will 1.2 moles helium occupy at the same temperature and pressure?

$$V_{2} = V_{1} \times \underline{n}_{2}$$

$$n_{1}$$

$$V_{2} = 1.5 \text{ L x} \quad \underline{1.2 \text{ moles He}}$$

$$0.75 \text{ mole He}$$

= 2.4L



Summary of Gas Laws

Law	Variable quantities	Constant quantities
Boyle's law	Pressure Volume	Temperature (K) Number of moles
Charles's law	Temperature (K) Volume	Pressure Number of moles
Avogadro's law	Number of moles Volume	Pressure Temperature (K)

Increasing or decreasing the volume of a gas at a constant temperature

Boyle's Law





5.4 The ideal gas equation

Ideal Gas Equation

Boyle's law: $V \alpha \frac{1}{P}$ (at constant *n* and *T*) Charles' law: $V \alpha T$ (at constant *n* and *P*) Avogadro's law: $V \alpha n$ (at constant *P* and *T*)

The **volume** of a gas is inversely proportional to **pressure** and directly proportional to **temperature** and the number of **moles** of molecules



R is the gas constant

- P = pressure (atm)
- V = volume (L)
- n = no. of moles (mol)
- R = ideal gas constant = 0.08206 (L atm K⁻¹ mol⁻¹)

T = temperature (K)

Ideal Gas

Ideal gas is a hypothetical gas whose pressurevolume-temperature behavior can be completely accounted for by the ideal gas equation

At 0 °C and 1 atm pressure, many real gases behave like an ideal gas



Standard Temperature and Pressure (STP)

The conditions 0 °C (273.15 K) and 1 atm are called **standard temperature and pressure (STP).**

Experiments show that at STP, 1 mole of an ideal gas occupies 22.414 L.

PV = nRT

$$R = \frac{PV}{nT} = \frac{(1 \text{ atm})(22.414\text{L})}{(1 \text{ mol})(273.15 \text{ K})}$$

 $R = 0.082057 L \cdot atm / (mol \cdot K)$ R = 0.0821 L $\cdot atm / (mol \cdot K)$



What is the volume (in liters) occupied by 49.8 g of HCl at STP?

$$T = 0 \ {}^{0}\text{C} = 273.15 \text{ K}$$

 $P = 1 \text{ atm}$
 $n = 49.8 \text{ g x} \frac{1 \text{ mol HCl}}{36.45 \text{ g HCl}} = 1.37 \text{ mol}$

$$PV = nRT$$

$$V = \frac{nRT}{P}$$

$$I.37 \mod x \ 0.0821 \ \frac{\text{Leatm}}{\text{motor}} \ x \ 273.15 \text{ K}$$

$$V = \frac{1.37 \mod x \ 0.0821}{1 \text{ atm}}$$

$$V = 30.7 \text{ L}$$

Molar Volume (V_m) At STP (T= 273.15 K, P= 1 atm), 1 mole of a gas occupies a volume of 22.41 L (molar volume).



TABLE 5.1Volume Occupied by 1 mol of Several Different Gasesat 0°C and 1 atm Pressure

Gas	Formula	Formula mass (amu)	Volume (L)*
hydrogen	H_{2}	2.016	22.43
helium	He	4.003	22.42
nitrogen	N ₂	28.02	22.38
carbon monoxide	CÔ	28.01	22.38
oxygen	O ₂	32.00	22.40

*The volumes are expressed to four significant figures to show the variability that accompanied these experimentally determined values.

Using Molar Volume

Moles of gas

Molar volume 22.4 L/mol

Volume (L) of gas

What is the volume occupied by 2.75 moles N_2 gas at STP? 2.75 moles $N_2 \times \frac{22.41 \text{ L}}{1 \text{ mole}} = 61.63 \text{ L}$

How many grams of He are present in 8.00 L of gas at STP?

8.00 L x <u>1 mole He</u> x <u>4.00 g He</u> = 1.43 g He 22.41 L 1 mole He

Combined Gas Law

$$PV = nRT$$

 $\frac{PV}{nT} = R$

 $\frac{P_1 V_1}{n_1 T_1} = \frac{P_2 V_2}{n_2 T_2}$

The combined gas law uses Boyle's Law, Charles' Law, and Avogadro's Law Argon is an inert gas used in lightbulbs to retard the vaporization of the filament. A certain lightbulb containing argon at 1.20 atm and 18 °C is heated to 85 °C at constant volume. What is the final pressure of argon in the lightbulb (in atm)?



PV = *nRT n*, *V* and *R* are constant

- $\frac{nR}{V} = \frac{P}{T} = \text{constant} \qquad P_1 = 1.20 \text{ atm} \qquad P_2 = ?$ $T_1 = 291 \text{ K} \qquad T_2 = 358 \text{ K}$
 - $\frac{P_1}{T_1} = \frac{P_2}{T_2}$ $P_2 = P_1 x \frac{T_2}{T_1} = 1.20 \text{ atm } x \frac{358 \text{ K}}{291 \text{ K}} = 1.48 \text{ atm}$

A gas has a volume of 675 mL at 35°C and 646 mm Hg pressure. What is the volume(mL) of the gas at -95°C and a pressure of 802 mm Hg (n constant)?

 $T_1 = 308 \text{ K}$ $T_2 = -95^{\circ}\text{C} + 273 = 178\text{K}$ $V_1 = 675 \text{ mL}$ $V_2 = ???$ $P_1 = 646 \text{ mm Hg}$ $P_2 = 802 \text{ mm Hg}$

$$\frac{P_{1}}{T_{1}} \frac{V_{1}}{T_{1}} = \frac{P_{2}}{T_{2}} \frac{V_{2}}{T_{2}}$$

$$V_{2} = V_{1} \times \frac{P_{1}}{P_{2}} \times \frac{T_{2}}{T_{1}}$$

$$V_{2} = 675 \text{ mL } \times \frac{646 \text{ mm Hg } \times 178 \text{K}}{802 \text{ mm Hg } \times 308 \text{K}} = 314 \text{ mL}$$

Density (d) and Molar Mass (\mathcal{M}) Calculations



A 2.10-L vessel contains 4.65 g of a gas at 1.00 atm and 27.0 °C. What is the molar mass of the gas?



 \mathcal{M} = 54.5 g/mol

5.5 Gas Stoichiometry

Gas Stoichiometry

Calculation about amounts (moles) or volumes of reactants and products



What volume (L) of O_2 gas is needed to completely react with 15.0 g of aluminum at STP? $4 \operatorname{Al}(s) + 3 O_2(g) \longrightarrow 2 \operatorname{Al}_2O_3(s)$

mass of Al \rightarrow mole of Al \rightarrow mole of O₂ \rightarrow volume of O₂(STP)

 $15.0 \text{ g Al } x \underline{1 \text{ mole Al}} x \underline{3 \text{ moles O}_2} x \underline{22.41 \text{ L}} = 9.34 \text{ L O}_2$ $27.0 \text{ g Al} 4 \text{ moles Al} 1 \text{ mole O}_2$

What is the volume of CO₂ produced at 37 ^oC and 1.00 atm when 5.60 g of glucose are used up in the reaction: $C_6H_{12}O_6(s) + 6O_2(g) \longrightarrow 6CO_2(g) + 6H_2O(I)$ $g C_6 H_{12} O_6 \longrightarrow mol C_6 H_{12} O_6 \longrightarrow mol CO_2 \longrightarrow V CO_2$ 5.60 g C₆H₁₂O₆ x $\frac{1 \text{ mol } C_6 H_{12}O_6}{180 \text{ g } C_6 H_{12}O_6}$ x $\frac{6 \text{ mol } CO_2}{1 \text{ mol } C_6 H_{12}O_6} = 0.187 \text{ mol } CO_2$ $V = \frac{nRT}{P} = \frac{0.187 \text{ mol x } 0.0821 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{K}} \times 310.15 \text{ K}}{1.00 \text{ atm}} = 4.76 \text{ L}$

5.6 Dalton's Law of Partial Pressures



The partial pressure of a gas

•is the pressure of each gas in a mixture.

•is the pressure that gas would exert if it were by itself in the container.

Dalton's Law of Partial Pressures states that the total pressure of a gaseous mixture is equal to the sum of the individual pressures of each gas.

P1 + P2 + P3 + ... = P total

The pressure depends on the total number of gas particles, not on the types of particles.

Dalton's Law of Partial Pressures

Vand Tare constant



 P_1

 P_2

 $P_{\text{total}} = P_1 + P_2$

Typical composition of air

Gas	Partial Pressure (mm Hg)	Percentage (%)
Nitrogen, N ₂	594.0	78
Oxygen, O ₂	160.0	21
Carbon dioxide, CO ₂	0.3 }	1
Water vapor, H ₂ O	5.7 J	
Total air	760.0	100

 An atmospheric sample contains nitrogen, oxygen, and argon. If the partial pressure of nitrogen is 587 mm Hg, oxygen is 158 mm Hg, and argon is 7 mm Hg, what is the barometric pressure?

$$P_{\text{total}} = P_{\text{nitrogen}} + P_{\text{oxygen}} + P_{\text{argon}}$$
$$P_{\text{total}} = 587 \text{ mm Hg} + 158 \text{ mm Hg} + 7 \text{ mm Hg}$$
$$P_{\text{total}} = 752 \text{ mm Hg}$$

A scuba tank contains O_2 with a pressure of 0.450 atm and He at 855 mm Hg. What is the total pressure in mm Hg in the tank?

 $0.450 \text{ atm x } \frac{760 \text{ mm Hg}}{1 \text{ atm}} = 342 \text{ mm Hg} = P_{0_2}$

$$P_{\text{total}} = P_{O_2} + P_{\text{He}}$$

 $P_{\text{total}} = 342 \text{ mm Hg} + 855 \text{ mm Hg}$ = 1197 mm Hg Consider a case in which two gases, A and B, are in a container of volume V.

$$n_A$$
 is the number of moles of A



 $P_{A} = \frac{n_{A}RI}{V}$

 $n_{\rm B}$ is the number of moles of B



$$P_{\rm T} = P_{\rm A} + P_{\rm B}$$
 $X_{\rm A} = \frac{n_{\rm A}}{n_{\rm A} + n_{\rm B}}$ $X_{\rm B} = \frac{n_{\rm B}}{n_{\rm A} + n_{\rm B}}$

 $P_{\rm A} = X_{\rm A} P_{\rm T}$ $P_{\rm B} = X_{\rm B} P_{\rm T}$

$$P_i = X_i P_T$$

mole fraction (X_i) =
$$\frac{n_i}{n_T}$$

A sample of natural gas contains 8.24 moles of CH_4 , 0.421 moles of C_2H_6 , and 0.116 moles of C_3H_8 . If the total pressure of the gases is 1.37 atm, what is the partial pressure of propane (C_3H_8)?

$$P_i = X_i P_T$$
 $P_T = 1.37$ atm
 $X_{\text{propane}} = \frac{0.116}{8.24 + 0.421 + 0.116} = 0.0132$
 $P_{\text{propane}} = 0.0132 \times 1.37$ atm = 0.0181 atm



 $P_{\rm T} = P_{\rm O_2} + P_{\rm H_2O}$

5.7 Kinetic Molecular Theory of Gases



Kinetic Molecular Theory of Gases

This theory explains the behavior of gases

- Gases are composed of molecules that are separated by large distances. The molecules (" point ") possess mass but have negligible volume.
- 2. Gas molecules are in constant motion in random directions, and they frequently collide with one another. Collisions among molecules are perfectly elastic (energy can be transferred between molecules but no energy is gained or lost during collision).
- 3. Gas molecules exert neither attractive nor repulsive forces on one another.
- 4. Energy of motion is called kinetic energy (KE). The average KE of the molecules is proportional to absolute T. Any two gases at the same T will have the same average KE.

Kinetic Molecular Theory of Gases

- $\overline{KE} = \frac{1}{2} m \overline{u^2} \qquad m =$ $\overline{KE} \propto T \qquad u^2 =$ $\frac{1}{2}m \overline{u^2} \propto T \qquad C = p$ $\frac{1}{2}m \overline{u^2} = CT$
 - m = mass of the molecule
 - $u^{\overline{2}}$ = mean square speed
 - *C* = *proportionality constant*

... The T of a gas is a measure of the average KE of the molecules

Maxwell speed distribution curves

The distribution of gas molecule speeds at various temperature $\uparrow T$, \uparrow number of molecules moving at high speed


Root-mean-square (rms) speed (u_{rms})



Number of molecules

Gas diffusion is the gradual mixing of molecules of one gas with molecules of another by virtue of their kinetic properties.



a small opening.

5.8 Deviations from Ideal Behavior







Why real gases deviate from ideal behavior ??? At higher P, gas density 1, molecules are close together. Intermolecular forces (attractive force) exist and affect the motion of the molecules

In real gases, the molecules possess definite volume

Ideal gas (behave ideally) Real gas (behave non-ideally)



Van der Waals equation

This equation is a modification of the ideal gas equation. It accounts for the attractive forces and molecular volume

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

corrected pressure

corrected volume

a, b = constant

TABLE 5.4

van der Waals Constants of Some Common Gases

а		b
Gas	$\left(\frac{\text{atm}\cdot \text{L}^2}{\text{mol}^2}\right)$	$\left(\frac{\mathbf{L}}{\mathbf{mol}}\right)$
He	0.034	0.0237
Ne	0.211	0.0171
Ar	1.34	0.0322
Kr	2.32	0.0398
Xe	4.19	0.0266
H_2	0.244	0.0266
N_2	1.39	0.0391
O_2	1.36	0.0318
Cl_2	6.49	0.0562
CO_2	3.59	0.0427
CH_4	2.25	0.0428
CCl_4	20.4	0.138
NH_3	4.17	0.0371
H_2O	5.46	0.0305

Chapter 6 Thermochemistry

6.1 The nature of energy and types of energy
6.2 Energy changes in chemical reactions
6.3 Introduction to thermodynamics
6.4 Enthalpy
6.4 Calorimetry
6.5 Standard enthalpy of formation and reaction
6.6 Heat of solution and dilution

6.1 The nature of energy and types of energy





Energy is the capacity to do work. Work(w) = energy used to move an object over some distance = force x distance (F x d) $= 1 \text{ kgm}^{2}/\text{s}^{2}$ = 1 Nm= 1 JSI unit = **Joule (J)** One joule of work is done when a force of one Newton is applied over a distance of one metre Velocity (m/s) Acceleration (m/s²) Force = mass (kg) x acceleration (m/s^2)

= kgm/s²

Types of energy

• *Kinetic energy* is the energy of motion

Potential energy is the energy associated with an object's position

•*Radiant energy* comes from the sun and is earth's primary energy source

Thermal energy is the energy associated with the random motion of atoms and molecules

 Chemical energy is the energy stored within the bonds of chemical substances

•*Nuclear energy* is the energy stored within the collection of neutrons and protons in the atom

6.2 Energy changes in chemical reactions





Law of conservation of energy

- •Energy can converted from one form to another or transferred from one object to another.
- •Total amount of energy in the universe remains constant.
- •Energy cannot be created or destroyed.

Energy conversion

Chemical Motion Chemico

electrical energy to light energy to P thermal and radiant energy ki

Potential energy to kinetic energy

Energy Transformations

Almost all chemical reactions absorb/produce energy in the form of heat

Heat is the transfer of **thermal energy** (molecular motion) between two bodies that are at different temperatures (Heat flow)

Temperature is a measure of the thermal energy.

Temperature ¥ Thermal Energy

WHAT IS HEAT





100°C

System and Surroundings

System - the specific part of the universe that is of interest in the study. Systems usually include substances involved in chemical and physical changes.

Surroundings - the rest of the universe outside the system.



System and Surrounding



Surroundings (flask and subtances in contact with outside of flask)

System (contents)

Exothermic process is any process that gives off heat – transfers thermal energy from the system to the surroundings.



$$2H_2(g) + O_2(g) \longrightarrow 2H_2O(l) + energy$$
$$H_2O(g) \longrightarrow H_2O(l) + energy$$

Endothermic process is any process in which heat has to be supplied to the system from the surroundings.



energy + 2HgO (s)
$$\longrightarrow$$
 2Hg (\hbar + O₂ (g)
energy + H₂O (s) \longrightarrow H₂O (\hbar

Exothermic

Endothermic



energy of the products <
 energy of the reactants</pre>

energy of the products >
energy of the reactants

6.3 Introduction to thermodynamics



Thermochemistry is the study of heat change in chemical reactions. Thermochemistry is part of a broader subject called Thermodynamics.

Thermodynamic = scientific study of the interconversion of heat and other kinds of energy

State of a system = the values of all relevant macroscopic properties-example: energy, temperature, pressure, volume. State function

- properties that are determined by the state of the system (eg. energy, temp, pressure, volume).
- depends only on the initial and final states of the system, not on the path by which the system arrived at that state.

$$\Delta E = E_{\text{final}} - E_{\text{initial}} \quad \Delta V = V_{\text{final}} - V_{\text{initial}}$$

$$\Delta P = P_{final} - P_{initial} \quad \Delta T = T_{final} - T_{initial}$$

q and w are not state functions They are not properties of a system

 $\Delta q \times q_{final} - q_{initial}$

- Energy, E is a function of state-not easily measured.
- ΔE has a unique value between two states-easily measured.

 $\Delta E = E_{final} - E_{initial}$

Independent of the path by which the system achieved that state.

Potential energy of hiker 1 and hiker 2 is the same even though they took different paths.

First law of thermodynamics – energy can be converted from one form to another, but cannot be created or destroyed.

Change in internal energy, $\Delta E = E_{final} - E_{initial}$

Internal energy = Total energy (kinetic + potential) in a system Transfer of energy from the system to the surroundings does not change the total energy of the universe

$$\Delta E_{system} + \Delta E_{surroundings} = 0$$
$$\Delta E_{system} = -\Delta E_{surroundings}$$

Change of energy (ΔE)

When energy is exchanged between the system and the surroundings, it is exchanged as either heat (*q*) or work (*w*).

$\Delta \mathbf{E} = \mathbf{q} + \mathbf{w}$

Energy **lost** by the system = Energy **gained** by the surroundings



- ΔE = the change in internal energy of a system
- q = the heat exchange between the system and the surroundings
- w = the work done on (or by) the system

Sign conventions for & heat

$\Delta \mathbf{E} = \mathbf{q} + \mathbf{w}$

Process Sign Work done by the system on the surroundings Work done on the system by the surroundings +Heat absorbed by the system from the surroundings (endothermic process) Heat absorbed by the surroundings from the system (exothermic process) Surroundings Surroundings System System +q+wq -w**System loses heat** System gains heat Work done by system Work done on system

 $-\Delta E$ (loss of internal energy) $+\Delta E$ (gain of internal energy)

Work and Heat

$$w = F x d$$
 unit = J

 $\Delta V < 0$

.: w is positive

Mechanical work done by gas(reaction in vessel fitted with a piston)

P= constant external pressure



 $\Delta V > 0$

:: w is negative

A sample of nitrogen gas expands in volume from 1.6 L to 5.4 L at constant temperature. What is the work done in joules if the gas expands (a) against a vacuum and (b) against a constant pressure of 3.7 atm?

$$W = -P \Delta V$$

(a)
$$\Delta V = 5.4 L - 1.6 L = 3.8 L$$
 $P = 0$ atm
 $W = -0$ atm x 3.8 L = 0 L•atm = 0 joules
(b) $\Delta V = 5.4 L - 1.6 L = 3.8 L$ $P = 3.7$ atm

$$w = -3.7 \text{ atm x } 3.8 \text{ L} = -14.1 \text{ L} \cdot \text{atm}$$

 $w = -14.1 \text{ L} \cdot \text{atm x } \frac{101.3 \text{ J}}{1 \text{ L} \cdot \text{atm}} = -1430 \text{ J}$





(1 L. atm = 101.3 J)

6.4 Enthalpy



Enthalpy (H) (extensive property) is used to quantify the heat flow into or out of a system in a process that occurs at **constant pressure**.

Enthalpy = internal energy + product of pressure-volume

$$H = E + PV$$

$$\Delta H = \Delta E + P\Delta V \qquad P \text{ constant}$$

$$\Delta H = (q+w) - w \qquad \Delta E = q + w$$

$$\omega H = q \qquad w = -P \Delta V$$

Change of enthalpy of the system = heat flow into/out the system (heat gain/heat lost)

Enthalpy of reaction, $\Delta H = H$ (products) – H (reactants)



(Endothermic)

 $\Delta H < 0$ (Exothermic)



6.01 kJ are absorbed for every 1 mole of ice that melts at 0°C and 1 atm.

$$H_2O(s) \longrightarrow H_2O(l) \qquad \Delta H = 6.01 \text{ kJ/mol}$$



890.4 kJ are released for every 1 mole of methane that is combusted at 25°C and 1 atm.

 $CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(h) \Delta H = -890.4 \text{ kJ/mol}$

 The stoichiometric coefficients always refer to the number of moles of a substance

$$H_2O(s) \longrightarrow H_2O(h)$$

 $\Delta H = 6.01 \text{ kJ/mol}$

• If you reverse a reaction, the sign of ΔH changes

$$H_2O(h) \longrightarrow H_2O(s)$$

 $\Delta H = -6.01 \text{ kJ/mol}$



• If you multiply both sides of the equation by a factor n, then ΔH must change by the same factor n.

 $2H_2O(s) \longrightarrow 2H_2O(t) \quad \Delta H = 2 \times 6.01 = 12.0 \text{ kJ}$

• The physical states of all reactants and products must be specified in thermochemical equations.

$$H_2O(s) \longrightarrow H_2O(h) \qquad \Delta H = 6.01 \text{ kJ/mol}$$
$$H_2O(h) \longrightarrow H_2O(g) \qquad \Delta H = 44.0 \text{ kJ/mol}$$

How much heat is evolved when 266 g of white phosphorus (P_4) burn in air?

 $P_4(s) + 5O_2(g) \longrightarrow P_4O_{10}(s) \quad \Delta H = -3013 \text{ kJ/mol}$

266 g
$$P_4 \times \frac{1 \text{ mol } P_4}{123.9 \text{ g } P_4} \times \frac{3013 \text{ kJ}}{1 \text{ mol } P_4} = 6470 \text{ kJ}$$



Calorimetry = measurement of heat change

The *specific heat* (s) of a substance is the amount of heat (q) required to raise the temperature of **one gram** of the Unit = $J/g \cdot {}^{\circ}C$ substance by **one degree** Celsius.

The *heat capacity* (C) of a substance is the amount of heat (q) required to raise the temperature of a given quantity (m) of the substance by **one degree** Celsius. Unit = $J/^{\circ}C$

> Specific Heat (J/g · °C) Substance A1 0.900 0.129 Au C (graphite) 0.720 C (diamond) 0.502 Cu 0.385 Fe 0.4440.139 Hg H₂O 4.184 C_2H_5OH (ethanol) 2.46

Heat (*q*) absorbed or released:

$$q = C\Delta t \qquad \Delta t = t_{\text{final}} - t_{\text{initial}}$$
$$q = ms\Delta t$$

q > 0 = endothermic process q < 0 = exothermic process

m	S

Determine the heat capacity for 60.0g of water.

A 466g sample of water is heated from 8.50 °C to 74.60 °C. Calculate the amount of heat absorbed by the water in kJ.

q = ms∆t

q = (466g)(4.184 J/g[.]°C)(74.60 °C - 8.50 °C)

q = 128878 J

q = 129 kJ

How much heat is given off when an 869 g iron bar cools from 94°C to 5°C?

s of Fe = 0.444 J/g \cdot °C

$$\Delta t = t_{\text{final}} - t_{\text{initial}}$$

= 5°C - 94°C = -89°C

 $q = ms \Delta t$

- = 869 g x 0.444 J/g °C x –89°C
- = -34,000 J = -34 kJ
Constant-Volume Calorimetry ("Bomb" calorimeter)



No heat/mass enters/leaves (isolated system)

Constant-Pressure Calorimetry ("coffee-cup" calorimeter)



No heat enters or leaves!

measure heat of reactions (acid-base neutralization, heat of solution, heat of dilution)



 $q_{rxn} = -(q_{water} + q_{cal})$ $q_{water} = ms\Delta t$ $q_{cal} = C_{cal}\Delta t$

Reaction at Constant P $\Delta H = q_{rxn}$

TABLE 6.3 Heats of Some Typical Reactions Measured at Constant Pressure

Type of Reaction	Example	∆ <i>H</i> (kJ/mol)
Heat of neutralization	$\text{HCl}(aq) + \text{NaOH}(aq) \longrightarrow \text{NaCl}(aq) + \text{H}_2\text{O}(l)$	-56.2
Heat of ionization	$H_2O(l) \longrightarrow H^+(aq) + OH^-(aq)$	56.2
Heat of fusion	$H_2O(s) \longrightarrow H_2O(l)$	6.01
Heat of vaporization	$H_2O(l) \longrightarrow H_2O(g)$	44.0*
Heat of reaction	$MgCl_2(s) + 2Na(l) \longrightarrow 2NaCl(s) + Mg(s)$	-180.2

*Measured at 25°C. At 100°C, the value is 40.79 kJ.

Because no heat enters or leaves the system throughout the process, heat lost by the reaction must be equal to the heat gained by the calorimeter and water, therefore, we can write...



where q_{water} is determined by $q = ms \Delta t$ and $q_{calorimeter}$ is determined by $q = C\Delta t$

A reactant was burned in a constant-volume calorimeter. The temperature of the water increased from 20.17 °C to 25.84 °C. Given the mass of water surrounding the calorimeter is 2000g and the heat capacity of the calorimeter is1.80 kJ/ °C, calculate the heat of combustion.

heat lost by the reaction = heat gained by the water and bomb

$$\mathbf{q} = -(\mathbf{q}_{water} + \mathbf{q}_{cal})$$

q_{water} = ms∆t

- = (2000g)(4.184J/g. °C)(25.84 °C 20.17 °C)
- = 47400 J or 47.4 kJ

 $\mathbf{q}_{bomb} = \mathbf{C} \Delta \mathbf{t}$

= (1.80 kJ/°C)(25.84 °C - 20.17 °C)

= 10.2 kJ

- $\mathbf{q} = -(\mathbf{q}_{water} + \mathbf{q}_{cal})$
- q = -(47.4 kJ + 10.2 kJ) = -57.6 kJ

6.5 Standard enthalpy of formation and reaction

Absolute enthalpy cannot be determined. H is a state function so changes in enthalpy, ΔH , have unique values.

Standard enthalpy of formation (ΔH_{f}^{0}) is the heat change for the formation of **one mole** of a compound from its **elements** at standard conditions (1 atm & 25°C)

The standard enthalpy of formation of any element in its most stable form is zero.

 $\Delta H^{0}_{f}(O_{2}) = 0$ $\Delta H^{0}_{f}(O_{3}) = 142 \text{ kJ/mol}$ $\Delta H^{0}_{f}(C, \text{ graphite}) = 0$ $\Delta H^{0}_{f}(C, \text{ diamond}) = 1.90 \text{ kJ/mol}$





TABLE 6.4	Standard Enthalpies of Formation of Some Inorganic
	Substances at 25°C

Substance	$\Delta H_{\rm f}^{\circ}$ (kJ/mol)	Substance	Δ <i>H</i> [°] _f (kJ/mol)
$\overline{\mathrm{Ag}(s)}$	0	$H_2O_2(l)$	-187.6
AgCl(s)	-127.0	Hg(l)	0
Al(s)	0	$I_2(s)$	0
$Al_2O_3(s)$	-1669.8	HI(g)	25.9
$\operatorname{Br}_2(l)$	0	Mg(s)	0
HBr(g)	-36.2	MgO(s)	-601.8
C(graphite)	0	$MgCO_3(s)$	-1112.9
C(diamond)	1.90	$N_2(g)$	0
CO(g)	-110.5	$NH_3(g)$	-46.3
$CO_2(g)$	-393.5	NO(g)	90.4
Ca(s)	0	$NO_2(g)$	33.85
CaO(s)	-635.6	$N_2O(g)$	81.56
$CaCO_3(s)$	-1206.9	$N_2O_4(g)$	9.66
$\operatorname{Cl}_2(g)$	0	O(g)	249.4
HCl(g)	-92.3	$O_2(g)$	0
Cu(s)	0	$O_3(g)$	142.2
CuO(s)	-155.2	S(rhombic)	0
$F_2(g)$	0	S(monoclinic)	0.30
HF(g)	-271.6	$SO_2(g)$	-296.1
H(g)	218.2	$SO_3(g)$	-395.2
$H_2(g)$	0	$H_2S(g)$	-20.15
$H_2O(g)$	-241.8	Zn(s)	0
$H_2O(l)$	-285.8	ZnO(s)	-348.0

The standard enthalpy of reaction (ΔH_{rxn}^0) is the enthalpy of a reaction carried out at 1 atm.

$$aA + bB \longrightarrow cC + dD$$

$$\Delta H_{rxn}^{0} = \left[\mathcal{C} \Delta H_{f}^{0} \left(C \right) + \mathcal{A} \Delta H_{f}^{0} \left(D \right) \right] - \left[\mathcal{A} \Delta H_{f}^{0} \left(A \right) + \mathcal{B} \Delta H_{f}^{0} \left(B \right) \right]$$

$\Delta H_{rxn}^0 = \Sigma n \Delta H_f^0$ (products) - $\Sigma m \Delta H_f^0$ (reactants)

ΔH^0 can be determined using the direct method or the indirect method.

The Direct Method for Determining ΔH^{0}

• Calculation of the enthalpy of formation of solid calcium oxide.

 $CaO(s) + CO_2(g) \longrightarrow CaCO_3(s)$ $\Delta H^{\circ}_{r\times n} = -177.8 \text{ kJ/mol}$

 $\Delta H^{\circ}_{r \times n} = \Sigma n \Delta H^{\circ}_{f}(products) - \Sigma n \Delta H^{\circ}_{f}(reactants)$

-177.8 kJ/mol = 1 mol(-1206.9) - [1 mol(x) + 1 mol(-393.5)]

$$\Delta H_{f^{\circ}}$$
 for CaO(s) = -635.6 kJ

The Indirect Method for Determining ΔH^0

Based on the law of heat summation (Hess's law).

Hess's Law: When reactants are converted to products, the change in enthalpy is the same whether the reaction takes place in one step or in a series of steps.

Enthalpy is a state function. It doesn't matter how you get there, only where you start and end (initial and final state)



Hess's Law

the ΔH for the overall process is the sum of the ΔH for the individual steps.

 $C(graphite) + O_2(g)$ $\Delta H^\circ = -110.5 \text{ kJ}$ $CO(g) + \frac{1}{2}O_2(g)$ Enthalpy $\Delta H^{\circ} =$ -393.5 kJ $\Delta H^{\circ} = -283.0 \text{ kJ}$ $CO_2(g)$

C (graphite) + $1/2O_2(g) \longrightarrow CO(g)$ <u>CO(g) + $1/2O_2(g) \longrightarrow CO_2(g)$ </u> C (graphite) + $O_2(g) \longrightarrow CO_2(g)$

Indirect method (Hess's Law) $S(s) + O_2(g) \rightarrow SO_2(g); \Delta H^\circ = -297 \text{ kJ}$ $2SO_3(g) \rightarrow 2SO_2(g) + O_2(g); \Delta H^\circ = 198 \text{ kJ}$ $2S(s) + 3O_2(g) \rightarrow 2SO_3(g); \Delta H^\circ = ?$

Answer :

 $2S(s) + 2O_{2}(g) \rightarrow 2SO_{2}(g); \Delta H^{o} = (-297 \text{ kJ}) \times (2)$ $2SO_{2}(g) + O_{2}(g) \rightarrow 2SO_{3}(g); \Delta H^{o} = (198 \text{ kJ}) \times (-1)$

 $2S(s) + 3O_2(g) \rightarrow 2SO_3(g); \Delta H^o = -792 kJ$

$$NO(g) \rightarrow \frac{1}{2}N_{2}(g) + \frac{1}{2}O_{2}(g) \Delta H = -90.25 \text{ kJ}$$

$$NO(g) + \frac{1}{2}O_{2}(g) \rightarrow NO_{2}(g) \Delta H = -57.07 \text{ kJ}$$

$$\frac{1}{2}N_{2}(g) + O_{2}(g) \rightarrow NO_{2}(g) \Delta H =??$$

$$\frac{1}{2}N_{2}(g) + \frac{1}{2}O_{2}(g) \rightarrow NO(g) \quad \Delta H = +90.25 \text{ kJ}$$

$$\frac{NO(g) + \frac{1}{2}O_{2}(g)}{\Delta H^{\circ} = -57.07 \text{ kJ}}$$

$$\frac{1}{2}N_{2}(g) + O_{2}(g) \rightarrow NO_{2}(g) \quad \Delta H = +33.18 \text{ kJ}$$

$$\frac{NO(g) + \frac{1}{2}O_{2}(g)}{\Delta H^{\circ} = -57.07 \text{ kJ}}$$

$$\frac{\Delta H^{\circ} = -57.07 \text{ kJ}}{\Delta H^{\circ} = +90.25 \text{ kJ}}$$

$$\frac{NO_{2}(g)}{\Delta H^{\circ} = +33.18 \text{ kJ}}$$

Benzene (C_6H_6) burns in air to produce carbon dioxide and liquid water. How much heat is released per mole of benzene combusted? The standard enthalpy of formation of benzene is 49.04 kJ/mol.

$$\frac{2C_{6}H_{6}(h + 15O_{2}(g) \longrightarrow 12CO_{2}(g) + 6H_{2}O(h)}{\Delta H_{rxn}^{0} = \Sigma n\Delta H_{f}^{0}(\text{products}) - \Sigma m\Delta H_{f}^{0}(\text{reactants})}$$

$$\Delta H_{rxn}^{0} = [12\Delta H_{f}^{0}(CO_{2}) + 6\Delta H_{f}^{0}(H_{2}O)] - [2\Delta H_{f}^{0}(C_{6}H_{6})]$$

$$\Delta H_{rxn}^{0} = [12x - 393.5 + 6x - 187.6] - [2x49.04] = -5946 \text{ kJ}$$

$$\frac{-5946 \text{ kJ}}{2 \text{ mol}} = -2973 \text{ kJ/mol } C_{6}H_{6}$$

45

6.6 Heat of solution and dilution



The *enthalpy/heat of solution* (ΔH_{soln}) is the heat generated or absorbed when a certain amount of solute dissolves in a certain amount of solvent.

$$\Delta H_{\rm soln} = H_{\rm soln} - H_{\rm components}$$

The *heat of dilution* is the heat change associated with the dilution process.

Heats of Solution of Some Ionic Compounds

Compound	∆H _{soln} (kJ/mol)
LiCl	-37.1
$CaCl_2$	-82.8
NaCl	4.0
KCl	17.2
NH ₄ Cl	15.2
NH ₄ NO ₃	26.2

Lattice energy (U)

 the energy required to completely separate one mole of a solid ionic compound into gaseous ions

Heat of hydration (ΔH_{hydr})

= the enthalpy change associated with the hydration process

Lattice energy (U)









7.1 FROM CLASSICAL PHYSICS TO QUANTUM THEORY
7.2 THE PHOTOELECTRIC EFFECT
7.3 BOHR'S THEORY OF THE HYDROGEN ATOM
7.4 THE DUAL NATURE OF THE ELECTRON
7.5 QUANTUM NUMBERS
7.6 ELECTRON CONFIGURATION
7.9 THE BUILDING-UP PRINCIPLE

Properties of Waves



Wave is the vibrating disturbance by which energy is transmitted. *Wavelength* (λ) is the distance between identical points on successive waves. Unit= m/cm/nm.

Amplitude is the vertical distance from the midline of a wave to the peak or trough.

Frequency (v) is the number of waves that pass through a particular point in 1s. Unit= Hz. (1Hz = 1 cycle/s).

Speed of the wave (u) = λv

Maxwell's Electromagnetic Radiation Theory

Light consists of **electromagnetic waves** (electric +magnetic)

Electromagnetic radiation is the emission and transmission of energy in the form of electromagnetic waves.

Speed of light (*c*) = λv

 $= 3.00 \times 10^8 \text{ m/s}$ Electric field component Magnetic field component

Types of electromagnetic radiation



A photon has a frequency of 6.0 x 10⁴ Hz. Convert this frequency into wavelength (nm).

$$\begin{split} \lambda &v = c \\ \lambda &= c/v \\ \lambda &= 3.00 \text{ x } 10^8 \text{ m/s} \text{ / } 6.0 \text{ x } 10^4 \text{ Hz} \\ \lambda &= 3.00 \text{ x } 10^8 \text{ m/s} \text{ / } 6.0 \text{ x } 10^4 \text{ /s} \\ \lambda &= 5.0 \text{ x } 10^3 \text{ m} \\ \lambda &= 5.0 \text{ x } 10^{12} \text{ nm} \end{split}$$

.

Planck's Quantum Theory

• When solids are heated, they emit electromagnetic radiation over a wide range of wavelengths.

•Atoms emit/absorb energy only in discrete units (quantum)

Quantum = the smallest quantity of energy that can be emitted/absorbed in the form of electromagnetic radiation.



7.2 THE PHOTOELECTRIC EFFECT





Light has both wave and particle-like properties

When sodium is bombarded with highenergy electrons, X rays are emitted. Calculate the energy (in joules) associated with the photons if the wavelength of the X rays is 0.154 nm.



$$E = h_V$$

 $E = h \times c / \lambda$

 $E = 6.63 \times 10^{-34} (J \cdot s) \times 3.00 \times 10^{8} (m/s) / 0.154 \times 10^{-9} (m)$ $E = 1.29 \times 10^{-15} J$



LIGHT IS A

7.3 BOHR'S THEORY OF THE HYDROGEN ATOM



Emission spectra

Continuous/line spectra of radiation emitted by substances
Every element has a unique emission spectrum.

continuous spectra = light emission at all wavelengths, eg sun, heated solid



line spectra = light emission only at specific wavelengths, eg H atom





Line Emission Spectrum of Hydrogen Atoms





Bohr's Theory of Atom

•explained the line spectrum of H postulated a "solar system" model (e⁻ travel in circular orbits around the nucleus)

- 1. e⁻ have specific (quantized) energy level
- 2. light is emitted as e⁻ moves from higher energy orbit to a lower-energy orbit

 $E_n = -R_{\rm H} \left(\frac{1}{n^2} \right)$

- $R_{\rm H}$ = Rydberg constant $= 2.18 \times 10^{-18} J$
- *n* = principal quantum number = 1,2,3,...

Ground level = lowest energy level(n=1) **Excited level** = higher energy level than ground level (n=2,3,...)



Electron



 $E_{\rm photon} = \Delta E = E_{\rm f} - E_{\rm i}$ $E_f = -R_H \left(\frac{1}{n_f^2} \right)$ $E_i = -R_{\rm H} \left(\frac{1}{n_i^2} \right)$ $\Delta E = R_{\rm H} \left(\frac{1}{n^2} - \frac{1}{n^2} \right)$ $\Delta E = hv = R_{\rm H} \left(\frac{1}{\rho_{i}^{2}} - \frac{1}{\rho_{i}^{2}}\right)$ $n_i > n_f$ ΔE -ve **Energy** lost (photon emitted)
Calculate the wavelength (in nm) of a photon emitted by a hydrogen atom when its electron drops from the n = 5 state to the n = 3 state.

$$E_{\text{photon}} = \Delta E = R_{\text{H}} \left(\frac{1}{n_{i}^{2}} - \frac{1}{n_{f}^{2}} \right)$$

$$E_{\text{photon}} = 2.18 \times 10^{-18} \text{ J} \times (1/25 - 1/9)$$

$$E_{\text{photon}} = \Delta E = -1.55 \times 10^{-19} \text{ J}$$

$$E_{\text{photon}} = h \times c / \lambda$$

$$\lambda = h \times c / E_{\text{photon}}$$

$$\lambda = 6.63 \times 10^{-34} (J \cdot s) \times 3.00 \times 10^{8} (\text{m/s}) / 1.55 \times 10^{-19} J$$

$$\lambda = 1280 \text{ nm}$$

7.4 THE DUAL NATURE OF THE ELECTRON



De Broglie Relation

De Broglie postulated that e⁻ is both particle and wave.

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

u = velocity of e-

m = mass of e-



h in J⋅s *m* in kg *u* in (m/s) What is the de Broglie wavelength (in nm) associated with a 2.5 g Ping-Pong ball traveling at 15.6 m/s?

 $\lambda = h/mu$ $\lambda = 6.63 \times 10^{-34} / (2.5 \times 10^{-3} \times 15.6)$ $\lambda = 1.7 \times 10^{-32} m$ $\lambda = 1.7 \times 10^{-23} nm$

7.5 QUANTUM NUMBERS









Quantum numbers

Quantum numbers are a set of values that describes the state of an electron including its distance from the nucleus, the orientation and type of orbital where it is likely to be found, and its spin.

1)Principal quantum number (n)
2)Angular momentum quantum number (l)
3)Magnetic quantum number (m₁)
4)Spin quantum number (m_s)



Principal quantum number (n)

- Energy of an orbital
- distance of e⁻ from the nucleus
- n = 1, 2, 3, 4,
- n ↑ orbital energy ↑
 - distance of e- (in orbital) from nucleus ↑
 - orbital size ↑
 - orbital stability \downarrow





Angular momentum quantum number (I)

- Shape of an orbital
- Possible values = 0 to (n-1)

possible values = 0 1 2 3 4 5..... *n*-1 letter designation = s p d f g h.....

values of <mark>n</mark>	va	lues of l		orbitals			
1		0		1s			
2		0, 1		2s, 2p			
3	(), 1, 2		3 <mark>s</mark> , 3p, 3d			
shells	\rightarrow subs	shells	\rightarrow	orbitals			







<u>Magnetic quantum number (m_l)</u>

- Orientation of an orbital
- Possible values = -I,....,0,....,+I
- Possible values = (2I+1)
- Number of orbitals within a subshell with a particular I

within subshell l = 2, there are 5 orbitals corresponding to

the 5 possible values of $\mathcal{M}_{\ell}(-2, -1, 0, +1, +2)$ d orbitals come in sets of 5 (-2, -1, 0, +1, +2)p orbitals in sets of 3 (-1, 0, +1)s orbitals in sets of 1 (0) n= 2 I=1 m_I = -1, 0, **or** 1

3 orientations is space



n= 3 m₁ = -2, -1, 0, 1, **or** 2 l= 2

5 orientations is space



Electron spin quantum number (m_s)

- Spinning motion of e-
- Possible values = +1/2 or -1/2





Atomic orbital



Energy of Orbitals in a single e- atom Eg. orbitals energy levels in H atom



 \rightarrow Energy only depends on principal quantum number *n*

Energy of orbitals in a multi-electron atom (atom containing two Eg. orbitals energy levels in many-electron atom or more e-)



\rightarrow depend on n & I

•e- will fill orbitals by the sum of *n* and *l*.

•Orbitals with equal values of (*n*+*I*) will fill with the lower *n* values first.

Order of orbitals (filling) in multi-electron atom

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



7.8 ELECTRON CONFIGURATION



Electron configuration of an atom = how the e- are distributed among various atomic orbitals in an atom



Quantum numbers: (n, l, m_{h}, m_{s})

Each electron's quantum numbers are unique and cannot be shared by another electron in that atom.

Pauli exclusion principle - no two electrons in an atom can have identical values of all 4 quantum numbers

s orbitals have 1 possible value of m_l to hold 2 electrons p orbitals have 3 possible value of m_l to hold 6 electrons d orbitals have 5 possible value of m_l to hold 10 electrons f orbitals have 7 possible value of m_l to hold 14 electrons

 \rightarrow : maximum of 2 electrons per orbital

atomic number (Z) = # protons = # electrons (in neutral atom)

He $1 s^{2}$ a single orbital can hold a "pair" of e- with opposite "spins" a single e- in an orbital is called "unpaired" Li $1 s^{2}$ $2 s^{1}$

Paramagnetism and Diamagnetism

- atoms with 1 or more *unpaired electrons are paramagnetic*, (attracted by a magnetic)
- atoms with all spins *paired are diamagnetic* (repelled by magnet)



Hund's Rule

- the most stable arrangement of electrons in subshells is the one with the greatest number of parallel spins.

e- configuration of C (Z=6)



Atom	Electron Configuration
н	1s ¹
He	1s ²
Li	1s ² 2s ¹
Be	1s ² 2s ²
В	1s ² 2s ² 2p ¹
С	1s ² 2s ² 2p ²
Ν	1s ² 2s ² 2p ³
0	1s ² 2s ² 2p ⁴
F	1s ² 2s ² 2p ⁵
Ne	1s ² 2s ² 2p ⁶
	Atom H He Li Be B C N C N O F

 $\uparrow \downarrow$

 $2s^2$

 $\uparrow \downarrow$

 $1s^2$

Ne

[Ne]

 $\uparrow \downarrow$

 $\uparrow \downarrow$

 $\uparrow\downarrow$

 $2p^6$



How many electrons can a 3rd shell (n=3) have ?

the 3rd shell (n = 3) can hold a maximum of 18 electrons:

<i>n</i> = 3	$\ell =$	0	1	2
	subshell	3 <mark>s</mark>	3 p	3 <i>d</i>
	# orbitals	1	3	5
	# electrons	2	6	10 = 18 total

Or use formula $2n^2$

How many 2*p* orbitals are there in an atom?



How many electrons can be placed in the 3d subshell?

If
$$l = 2$$
, then $m_l = -2$, -1 , 0 , $+1$, or $+2$
 $3d$ 5 orbitals which can hold a total of $10 e^{-1}$
 $1 = 2$

Determine the electron configuration of silicon

Silicon has 14 protons and 14 electrons

$$\frac{\uparrow\downarrow}{1s} \xrightarrow{\uparrow\downarrow}{2s} \xrightarrow{\uparrow\downarrow}{2p} \xrightarrow{\uparrow\downarrow}{3s} \xrightarrow{\uparrow}{\frac{\uparrow}{3p}} \xrightarrow{\uparrow}{3p}$$

The electron configuration of silicon is 1s²2s²2p⁶3s²3p²

7.9 THE BUILDING-UP PRINCIPLE



The Aufbau principle (building-up)

- e- are added progressively to the atomic orbitals to build up the element
- e- configuration of element are normally represented by a noble gas core

[Ne] =1s²2s²2p⁶ [Ar] =1s²2s²2p⁶3s²3p⁶ \rightarrow [Ne] 3s¹ \rightarrow [Ne] 3s¹

- The aufbau principle works for nearly every element tested.
- There are exceptions to this principle, eg chromium and copper

Cr (Z=24), the e- configuration is [Ar] $4s^13d^5$ instead of [Ar] $4s^23d^4$ Cu (Z=29), the e- configuration is [Ar] $4s^13d^{10}$ instead of [Ar] $4s^23d^9$

Because of greater stability associated with half-filled (3d⁵)and completely filled (3d¹⁰)subshells

What is the electron configuration of Mg?

Mg 12 electrons 1s < 2s < 2p < 3s < 3p < 4s $1s^22s^22p^63s^2$ 2 + 2 + 6 + 2 = 12 electrons Abbreviated as [Ne]3s² [Ne] =1s^22s^22p^6

What are the possible quantum numbers for the last (outermost) electron in CI?

Cl 17 electrons 1s < 2s < 2p < 3s < 3p < 4s $1s^22s^22p^63s^23p^5$ 2 + 2 + 6 + 2 + 5 = 17 electrons Last electron added to 3p orbital

n = 3 /= 1 $m_{1} = -1$, 0, or +1 $m_{s} = \frac{1}{2}$ or $-\frac{1}{2}$

ATOMIC		ELECTRON	ATOMIC		ELECTRON	ATOMIC		ELECTRON
NUMBER	SYMBOL	CONFIGURATION	NUMBER	SYMBOL	CONFIGURATION	NUMBER	SYMBOL	CONFIGURATION
1	Н	$1s^{1}$	37	Rb	[Kr]5s ¹	73	Та	[Xe]6s ² 4f ¹⁴ 5d ³
2	He	$1s^{2}$	38	Sr	[Kr]5s ²	74	W	[Xe]6s ² 4f ¹⁴ 5d ⁴
3	Li	[He]2s ¹	39	Y	[Kr]5s ² 4d ¹	75	Re	[Xe]6s ² 4f ¹⁴ 5d ⁵
4	Be	[He]2s ²	40	Zr	[Kr]5s ² 4d ²	76	Os	[Xe]6s ² 4f ¹⁴ 5d ⁶
5	В	[He]2s ² 2p ¹	41	Nb	[Kr]5s ¹ 4d ⁴	77	Ir	[Xe]6s ² 4f ¹⁴ 5d ⁷
6	С	[He]2s ² 2p ²	42	Mo	[Kr]5s ¹ 4d ⁵	78	Pt	[Xe]6s ¹ 4f ¹⁴ 5d ⁹
7	N	[He]2s ² 2p ³	43	Tc	[Kr]5s ² 4d ⁵	79	Au	[Xe]6s ¹ 4f ¹⁴ 5d ¹⁰
8	0	[He]2s ² 2p ⁴	44	Ru	[Kr]5s ¹ 4d ⁷	80	Hg	[Xe]6s ² 4f ¹⁴ 5d ¹⁰
9	F	[He]2s ² 2p ⁵	45	Rh	[Kr]5s ¹ 4d ⁸	81	Tl	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ¹
10	Ne	[He]2s ² 2p ⁶	46	Pd	[Kr]4d ¹⁰	82	Pb	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ²
11	Na	[Ne]3s ¹	47	Ag	[Kr]5s ¹ 4d ¹⁰	83	Bi	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ³
12	Mg	[Ne]3s ²	48	Cd	[Kr]5s ² 4d ¹⁰	84	Po	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁴
13	Al	[Ne]3s ² 3p ¹	49	In	[Kr]5s ² 4d ¹⁰ 5p ¹	85	At	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁵
14	Si	[Ne]3s ² 3p ²	50	Sn	[Kr]5s ² 4d ¹⁰ 5p ²	86	Rn	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 6p ⁶
15	Р	[Ne]3s ² 3p ³	51	Sb	[Kr]5s ² 4d ¹⁰ 5p ³	87	Fr	[Rn]7s ¹
16	S	[Ne]3s ² 3p ⁴	52	Te	[Kr]5s ² 4d ¹⁰ 5p ⁴	88	Ra	[Rn]7s ²
17	Cl	[Ne]3s ² 3p ⁵	53	I	[Kr]5s ² 4d ¹⁰ 5p ⁵	89	Ac	[Rn]7s ² 6d ¹
18	Ar	[Ne]3s ² 3p ⁶	54	Xe	[Kr]5s ² 4d ¹⁰ 5p ⁶	90	Th	[Rn]7s ² 6d ²
19	K	[Ar]4s ¹	55	Cs	[Xe]6s ¹	91	Pa	[Rn]7s ² 5f ² 6d ¹
20	Ca	[Ar]4s ²	56	Ba	[Xe]6s ²	92	U	[Rn]7s ² 5f ³ 6d ¹
21	Sc	[Ar]4s ² 3d ¹	57	La	[Xe]6s ² 5d ¹	93	Np	[Rn]7s ² 5f ⁴ 6d ¹
22	Ti	[Ar]4s ² 3d ²	58	Ce	$[Xe]6s^24f^15d^1$	94	Pu	[Rn]7s ² 5f ⁶
23	V	[Ar]4s ² 3d ³	59	Pr	[Xe]6s ² 4f ³	95	Am	[Rn]7s ² 5f ⁷
24	Cr	[Ar]4s ¹ 3d ⁵	60	Nd	[Xe]6s ² 4f ⁴	96	Cm	[Rn]7s ² 5f ⁷ 6d ¹
25	Mn	[Ar]4s ² 3d ⁵	61	Pm	[Xe]6s ² 4f ⁵	97	Bk	[Rn]7s ² 5f ⁹
26	Fe	[Ar]4s ² 3d ⁶	62	Sm	[Xe]6s ² 4f ⁶	98	Cf	[Rn]7s ² 5f ¹⁰
27	Co	[Ar]4s ² 3d ⁷	63	Eu	[Xe]6 <i>s</i> ² 4 <i>f</i> ⁷	99	Es	[Rn]7s ² 5f ¹¹
28	Ni	[Ar]4s ² 3d ⁸	64	Gd	[Xe]6s ² 4f ⁷ 5d ¹	100	Fm	[Rn]7s ² 5f ¹²
29	Cu	[Ar]4s ¹ 3d ¹⁰	65	Tb	[Xe]6s ² 4f ⁹	101	Md	[Rn]7s ² 5f ¹³
30	Zn	[Ar]4s ² 3d ¹⁰	66	Dy	[Xe]6s ² 4f ¹⁰	102	No	[Rn]7s ² 5f ¹⁴
31	Ga	[Ar]4s ² 3d ¹⁰ 4p ¹	67	Ho	[Xe]6s ² 4f ¹¹	103	Lr	[Rn]7s ² 5f ¹⁴ 6d ¹
32	Ge	[Ar]4s ² 3d ¹⁰ 4p ²	68	Er	[Xe]6s ² 4f ¹²	104	Rf	[Rn]7s ² 5f ¹⁴ 6d ²
33	As	[Ar]4s ² 3d ¹⁰ 4p ³	69	Tm	[Xe]6s ² 4f ¹³	105	На	[Rn]7s ² 5f ¹⁴ 6d ³
34	Se	[Ar]4s ² 3d ¹⁰ 4p ⁴	70	Yb	[Xe]6s ² 4f ¹⁴	106	Sg	[Rn]7s ² 5f ¹⁴ 6d ⁴
35	Br	[Ar]4s ² 3d ¹⁰ 4p ⁵	71	Lu	[Xe]6s ² 4f ¹⁴ 5d ¹	107	Ns	[Rn]7s ² 5f ¹⁴ 6d ⁵
36	Kr	[Ar]4s ² 3d ¹⁰ 4p ⁶	72	Hf	[Xe]6s ² 4f ¹⁴ 5d ²	108	Hs	[Rn]7s ² 5f ¹⁴ 6d ⁶
						109	Mt	[Rn]7s ² 5f ¹⁴ 6d ⁷

TABLE 7.3 The Ground-State Electron Configurations of the Elements*

Outermost subshell being filled with e-



•alkali metals and alkaline earth metals fill the s orbitals last

- main group elements fill the p orbitals last
- transition metals fill the d orbitals last
- lanthanides (4f) and actinides (5f) fill the f orbitals last



Chapter 8 Chemical Bonding I: Basic Concepts

- 9.1 Lewis dot symbols
- 9.2 the ionic bond
- 9.4 the covalent bond
- 9.5 Electronegativity
- 9.6 Writing Lewis structures
- 9.7 formal charge and Lewis structures
- ▶ 9.8 the concept of resonance
- 9.9 the exception of octate rules
9.1 Lewis dot symbols

- When atoms interact to form chemical bond, only their outer region are in contact
- The Octet Rule: in forming chemical bonds, atoms usually gain, lose or share electrons until they have 8 in the outer shell to reach the same electronic configuration of the noble gasses (ns² np⁶) (except hydrogen, helium and lithium).
- Lewis Dot Representation: In the representation of an atom, the valence electrons of an atom (outer most shell electrons) are represented by dots.
- There are two main types of chemical bonds: ionic bond and covalent bond.

Li Be B C N O F Ne

Lewis Dot Symbols



Table 9-1

Types of Bonds

Types of Atoms	Type of Bond	Bond Characteristic		
metals to	Ionio	electrons		
nonmetals	IOIIIC	transferred		
nonmetals to	Carralant	electrons		
nonmetals	Covalent	shared		

9.2 the ionic bond

• ionic bond is the electrostatic force that hold ions together in an ionic compound



- the resulting anions & cations attract each other in such a ratio that the charges cancel out.
- Note: Do not show the charges in the final product.
 Example: KI NOT K⁺I⁻

Example: $Ba^{+2} \& F^{-}$ - Need two negatives to neutralize +2 charge on barium ion: $Ba^{+2} F^{-1} F^{-1} = BaF_2$

• Use Lewis dot symbol to show formation of Al_2O_3



9.4 the covalent bond

• A covalent bond is a chemical bond in which two or more electrons are shared by two atoms.





or

Double bond - two atoms share two pairs of electrons





double bonds^{8e⁻ 8e⁻ 8e⁻}

Triple bond - two atoms share three pairs of electrons



Polar covalent bond or *polar bond* is a covalent bond with greater electron density around one of the two atoms







Comparing of the properties of covalent and ionic

- Covalent compounds are usually gases, liquid and low melting solid
- Ionic compounds are solids at room temperature and high melting point.
- Many ionic compounds are soluble in water , and the resulting aqueous solutions conduct electricity, because the compounds are strong electrolytes.

Electronegativity

- **Electronegativity** is the ability of an atom to attract toward itself the electrons in a chemical bond.
- High electronegativity \rightarrow pick up electron easily
- Electronegativity increase from left to right in period.
- Electronegativity increase from bottom to up in group.
- Transition metals don't follow these trend.

- Nonmetals have high electronegativity, metals have low electronegativity.
- high difference in electronegativity (2 or more), element tend to form ionic bond.(NaCl)
- small difference in electronegativity, element tend to form polar covelent bond .(HCl)

Same electronegative of the same elements form pure covelent bond (H_2)

Trends in electronegativity across a period The positively charged protons in the nucleus attract the negatively charged electrons. As the number of protons in the nucleus increases, the electronegativity or attraction will increase. Therefore electronegativity **increases** from **left to right** in a row in the periodic table. This effect only holds true for a row in the periodic table because the attraction between charges falls off rapidly with distance. The chart shows electronegativities from sodium to chlorine (ignoring argon since it does not does not form bonds).

Trends in electronegativity down a group As you go down a group, electronegativity decreases. (If it increases up to fluorine, it must decrease as you go down.) The chart shows the patterns of electronegativity in Groups 1 and 7.

The Electronegativities of Common Elements



Increasing electronegativity

Increasing electronegativity

Electron Affinity (EA) and electronegativity are related but in different concept

 \succ (EA) refers to isolated atoms attraction for additional electron (<u>experimental</u>)

 \geq EA \rightarrow <u>measurable</u>, Cl is highest

Electronegativity signifies the ability of an atom in a chemical bond(with another atom) to attract the shared electrons (estimated)

Electronegativity - <u>relative</u>, F is highest

Electron affinity is defined as the change in energy (in kJ/mole) of a neutral atom (in the gaseous phase) when an electron is added to the atom to form a negative ion. In other words, the neutral atom's likelihood of gaining an electron.

EXAMPLE 1: GROUP 1 ELECTRON AFFINITIES This trend of lower electron affinities for metals is described by the <u>Group 1</u> metals: Lithium (Li): 60 KJ mol⁻¹ Sodium (Na): 53 KJ mol⁻¹ Potassium (K): 48 KJ mol⁻¹ Rubidium (Rb): 47 KJ mol⁻¹ Cesium (Cs): 46 KJ mol⁻¹ Notice that electron affinity *decreases* down the group.

EXAMPLE 2: GROUP 17 ELECTRON AFFINITIES

For example, nonmetals like the elements in the halogens series in <u>Group 17</u> have a higher electron affinity than the metals. This trend is described as below. Notice the negative sign for the electron affinity which shows that energy is released.

Fluorine (F) –328 kJ mol⁻¹

Chlorine (Cl) –349 kJ mol⁻¹

Bromine (Br) –324 kJ mol⁻¹

lodine (I) –295 kJ mol⁻¹

Notice that electron affinity decreases down the group, but increases up with the period.

Variation of Electronegativity with Atomic Number



- Classify the following bonds as ionic, polar covalent, or covalent
- A) HCl =3-2.1=0.9
 Polar covalent
- b) KF =4-0.8=3.2
 lonic
- c) C-C =2.5-2.5=0
 covalent

- Classify the following bonds as ionic, polar covalent, or covalent
- A) CsCl =3-1=2 lonic
- ▶ b) H₂S = 2.5-2.1=0.4 Polar covalent
- ► c) N-N =3-3=0 Covalent

Nonpolarcovalent 0—0.3 Polar covalent 0.4—1.7 Ionic -greater than 1.8

9.6 Writing Lewis structures

- 1. Write the skeletal structure of the compounds, using chemical symbol and placing bonded atoms next to one another.
- determine the total number of electrons in the valence shells of all of the atoms of the molecule (A), add electrons (if molecule have net -ve charge, subtract electrons if molecule have net +ve charge)
- 3. Complete an octet for all atoms *except* hydrogen (B)
- 4. Find the number of bonds by C = B-A/2

5. Find the number of lone pair of electron by D = A - C

Writing Lewis Structures

A = 1X1 + 4X1 + 5X1 = 10 valance electrons



D=10-8=2 electrons

Lewis structure of HCN consist of 4 bond, 1 triple bond, 0 double bond, 2 nonbonding electrons or 1 pair of electrons

NH_4^+

- Step 2 A = 5X1 + 1X4 1 = 8 valance electrons
- Step 3 B = 8X1 + 2X4 = 16 electrons
- Step 4 C = 16-8 = 8/2=4 bonds
- Step 5 D= 8-8 = 0 non bonding electrons , 0 pair of electrons

Write the Lewis structure of nitrogen trifluoride (NF₃).

Step 1 – N is less electronegative than F, put N in center Step 2 – A= 5X1 + 7X3 = 26 valance electrons Step 3 – B = 8X1+8X3 = 32 electrons Step 4 – C = 32-26 = 6/2=3 bonds Step 5 – D= 26-6 = 20 nonbonding electrons or 10 pair of electrons



- Write the Lewis structure of carbon disulfide (CS_2) .
- Step 1 C is less electronegative than S, put C in center
- Step 2 A = 4X1 + 6X2 = 16 valance electrons
- Step 3 B = 8X1 + 8X2 = 24 electrons
- Step 4 C = 24-16 = 8/2=4 bonds
- Step 5 D= 16-8 =8 nonbonding electrons or 4 pair of electrons

S = C = S

- Write the Lewis structure of formic acid (HCOOH).
- Step 1 –put C in center ,surrounded by 2O atoms , H
- Step 2 A = 4X1 + 6X2 + 2x1 = 18 valance electrons
- Step 3 B = 8X1 + 8X2 + 2x2 = 28 electrons
- Step 4 C = 28-18 = 10/2=5 bonds
- Step 5 D= 18-10 = 8 nonbonding electrons or 4 pair of electrons

:O: || .. H -C- Q- H

- ▶ Write the Lewis structure of carbonate ion [CO₃]⁻²
- Step 1 C is less electronegative than O, put C in center
- Step 2 A = 4X1 + 6X3 + 2 = 24 valance electrons
- Step 3 B = 8X1 + 8X3 = 32 electrons
- Step 4 C = 32-24 = 8/2=4 bonds
- Step 5 D= 24-8 = 16 nonbonding electrons or 8 pair of electrons



- Write the Lewis structure of Nitrogen dioxide [NO₂]⁻¹
- Step 1 N is less electronegative than O, put N in center
- Step 2 A = 5X1 + 6X2 + 1 = 18 valance electrons
- Step 3 B = 8X1 + 8X2 = 24 electrons
- Step 4 C = $24-18 = \frac{6}{2} = 3$ bonds
- Step 5 D= 18-6 =12 nonbonding electrons or 6 pair of electrons

 $[: \dot{\mathbf{O}} - \dot{\mathbf{N}} = \dot{\mathbf{O}}:]^{-}$

9.7 formal charge and Lewis structures

• formal charge is the difference between the number of valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure.

formal charge on an _ of valence atom in a Lewis structure

total number electrons in the free atom

total number of nonbonding electrons

total number of bonding electrons



- For molecules , the sum of the charges should be zero
- For ion , the sum of the charges should be -ve for anions
- For ion , the sum of the charges should be +ve for cations
- formal charge and Lewis structures

- 1. For neutral molecules, a Lewis structure in which there are no formal charges is preferable to one in which formal charges are present.
- 2. Lewis structures with large formal charges are less plausible than those with small formal charges.
- 3. Among Lewis structures having similar distributions of formal charges, the most plausible structure is the one in which negative formal charges are placed on the more electronegative atoms



Which is the most likely Lewis structure for formaldehyde CH₂O



Which is the most likely Lewis structure for formaldehyde C,HN

H-C≡N:

• Write the formal charge for the carbonate ion?



 Write the formal charge for the NO₂⁻ ion?



9.8 the concept of resonance

- A **resonance structure** is one of two or more Lewis structures for a single molecule that cannot be represented accurately by only one Lewis structure (**after** formal charge has been determined).
- More possible structures gives the overall structure more validity.



Ozone



What are the resonance structures of the carbonate (CO_3^2 -) ion?



 Draw three resonance structure for N2O (NNO), indicate formal charge rank the structures.

- <u>1</u> :N=	+1 =N=	=Ö:	:N≡	+1 ≡N-	- <u>O</u> :	-2 ··· :N-	-N =	$\equiv \mathbf{O}$:
5	5	6.	5	5	6	5	5	6
6	4	6	_5	4	7	_7	4	5
-1	1	0	0	1	-1	-2	+1	+1

B > A > C

9.9 the exception of octate rules

- There are three types of ions or molecules that do not follow the octet rule:
 - Ions or molecules with an odd number of electrons
 - Ions or molecules with less than an octet (the incomplete Octet)
 - Ions or molecules with more than eight valence electrons (an expanded octet)

Ions or molecules with an odd number of electrons

 Though relatively rare and usually quite unstable and reactive, there are ions and molecules with an odd number of electrons(radical).

NO
$$N - 5e^-$$

 $O - 6e^-$
 $11e^-$

The incomplete Octet

 Covalent compounds containing Group 3 atoms may be satisfied with 6 valence electrons



An expanded octet

SF₆

- Usually occurs in element in 3rd period and beyond
 - More than 4 bonds
 - Elements \geq row 3 can use s, p & d orbitals and have > 8 VE

 PF_5

 XeF_4

- **P: 8 OR 10**
- **S**: 8, 10, OR 12
- **Xe: 8, 10, OR 12**
- Examples
Example 9-9

• Write Lewis structure AlI₃ Write Lewis structure BeF₂



Example 9-10

 Write Lewis structure PF₅



 Write Lewis structure AsF₅



Example 9-11

- Write Lewis structure
 [SO₄] ⁻²
 - :0: || :0-S-O: || :0:

 Write Lewis structure H₂SO₄

