University Of Anbar

College Of Engineering

CHEMISTRY

1st. stage

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LECTURE 1

MEASUREMENTS IN CHEMISTRY

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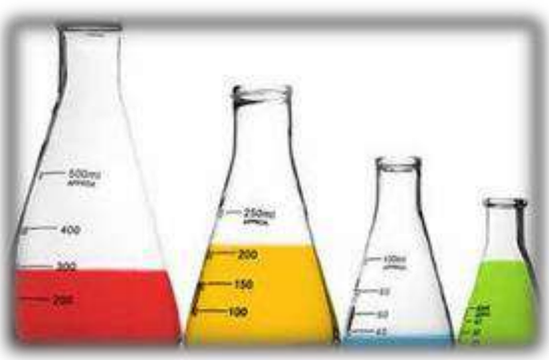
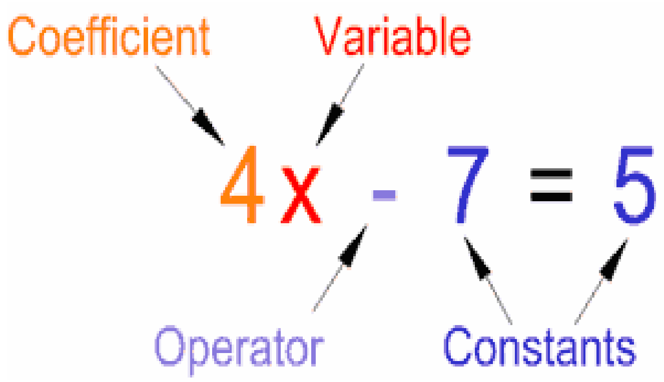




UNIT (1) MEASUREMENTS INCHEMISTRY

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 Systèm 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 conveniently represent very small or very large numbers. 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 7.5×10^{-3} (note the negative exponent).

The coefficient must always be a number greater than or equal to 1 but less than 10 or $1 \leq \text{coefficient} < 10$.

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) 4.0800×10^{2} (coefficient = 4.0800, exponent = +2)

b) 7.956×10^{-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

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
9.7×10^3	9.7 EE or EXP 3	9.7^{03} or 9.7E03 or 9700

Now try 8.1×10^{-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
8.1×10^{-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
↑	tera- (T)	10^{12} = 1,000,000,000,000
	giga- (G)	10^{9} = 1,000,000,000
	mega- (M)	10^{6} = 1,000,000
	kilo- (k)	10^{3} = 1,000
	deci- (d)	10^{-1} = 0.1
	centi- (c)	10^{-2} = 0.01
	milli- (m)	10^{-3} = 0.001
	micro- (μ)	10^{-6} = 0.000001
	nano- (n)	10^{-9} = 0.000000001
↓	pico- (p)	10^{-12} = 0.000000000001

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

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) 2.08×10^{-5} e) 600 f) 58.00

g) 4010049 h) 1.700×10^{2} i) 4.0100×10^{6}

Solution

	sf		sf		sf
0.0037	**2**	600.	**3**	93,000	**2**
2.08×10^{-5}	**3**	600	**1**	58.00	**4**
4010049	**7**	1.700×10^{2}	**4**	4.0100×10^{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

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.

Practice 1-4

Round off each of the following to three significant figures.

a) 9.174 b) 9.175 c) 9.176

d) 5 e) 0.0040 f) 8000

g) 2.4×10^{-5} h) 670

Answer

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 x 1.9483 b) $(2.50 \times 10^{-3}) \times (1.8500 \times 10^{5})$

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

Answer

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 b) 63.81 + 205.4

c) 191.000 - 188.0 d) 124.08 - 39.1740

e) $(6.8 \times 10^{-2}) + (2.04 \times 10^{-2})$ f) $(5.77 \times 10^{-4}) - (3.6 \times 10^{-4})$

Answer

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: $\frac{\text{umerator}}{\text{Denominator}}$ $\frac{1\ \text{g}}{2.20}$ or $\frac{2.20}{1\ \text{g}}$

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
	1Å = 10^{-10} 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 mL = 1 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		

Worked Example 1-3

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

a) 1 g = 1000 mg

b) 1 foot = 12 inches

c) 1 quart = 0.946 liter

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

Solution

Equality	Conversion factor	Conversion factor
1 g = 1000 mg	$\frac{1\text{ g}}{1000\text{ mg}}$	$\frac{1000\text{ mg}}{1\text{ g}}$
1 foot = 12 inches	$\frac{1\text{ ft.}}{12\text{ in.}}$	$\frac{12\text{ in.}}{1\text{ ft.}}$
1 quart = 0.946 liter	$\frac{1\text{ t.}}{0.\ 4}$	$\frac{0.\ 4}{1\text{ t.}}$
The accepted toxic dose of mercury is 0.30 mg per day.	$\frac{0.30\text{ mg}}{1\text{ da}}$	$\frac{1\text{ da}}{0.30\text{ mg}}$

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:

$$\frac{1\ \text{km}}{1000\ \text{m}} \quad \text{and} \quad \frac{1000\ \text{m}}{1\ \text{km}}$$

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

$$0.455\ \cancel{\text{km}} \times \frac{1000\ \text{m}}{1\ \cancel{\text{km}}} = 455\ \text{m}$$

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

$$4.5\ \cancel{\text{wk}} \times \frac{7\ \cancel{\text{d}}}{1\ \cancel{\text{wk}}} \times \frac{24\ \cancel{\text{h}}}{1\ \cancel{\text{d}}} \times \frac{60\ \text{min}}{1\ \cancel{\text{h}}} = 45000\ \text{min}$$

(45360 rounded to 2 sig figs.)

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)

$$\frac{2.7\ \cancel{\text{g}}}{1.0\ \cancel{\text{mL}}} \times \frac{1\ \text{lb}}{454\ \cancel{\text{g}}} \times \frac{1000\ \cancel{\text{mL}}}{1\ \text{L}} = 5.9\ \text{lb/L}$$

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.

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

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

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

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:

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

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

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

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

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.

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

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

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

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

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: $°C = \dfrac{(°F - 32)}{1.8}$

Celsius to Fahrenheit: $°F = 1.8\ °C + 32$

Celsius to Kelvin: $K = °C + 273$

Practice 1-10

Complete the following table.

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

Answer

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

utritionist use the word "Ca orie" (with a capita "C") to mean the same thing as kilocalorie.

1 **C**al = 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 cal = 4.184 J

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.

Specific Heats for Some Common Substances

	Substance	Specific Heat (J/g·°C)
Solids		
	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

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 = mass x specific heat x change in temperature*

$$q = m \times SH \times (T_{final} - T_{initial})$$

* The temperature change cou d a so e 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

$q = m \times SH \times \Delta T$

$q = 7.400\ g \times 4.18\ J/g{\cdot}°C \times 17.0°C = 526\ J$

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.

Answer

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.

Answer

Practice 1-13

4.00 x 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 J/g·°C.

Answer

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		
	7.28×10^{3}	
	3.608×10^{-5}	
	9.4090×10^{4}	
	1.5×10^{-3}	

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

a. 4.6 x 0.00300 x 193

b. 8.88 ÷ 99.40

c. $(7.120 \times 10^{-3}) \div (6.000 \times 10^{-5})$

d. $(5.92 \times 10^{3}) \times 3.87 \div 100$

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

a. 102 – 5.31 – 0.480

b. $(3.42 \times 10^{-4}) + (5.007 \times 10^{-4})$

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/cm^3 to lb/ft^3

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/cm^3. 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 cal/g·°C, how much heat is released?

Example for Lecture One

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. All trailing zeros that are placeholders are not significant.
3. Zeros between non zero numbers are significant.
4. All non zero numbers are significant.
5. 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.
6. 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 `433,000` unless changing the number into scientific notation.

Significant Figure Rules

There are three rules on determining how many significant figures are in a number:

1. Non-zero digits are always significant.
2. Any zeros between two significant digits are significant.
3. A final zero or trailing zeros in the decimal portion ONLY are significant.

Focus on these rules and learn them well. They will be used extensively throughout the remainder of this course. You would be well advised to do as many problems as needed to nail the concept of significant figures down tight and then do some more, just to be sure.

Please remember that, in science, all numbers are based upon measurements (except for a very few that are defined). Since all measurements are uncertain, we must only use those numbers that are meaningful. A common ruler cannot measure something to be 22.4072643 cm long. Not all of the digits have meaning (significance) and, therefore, should not be written down. In science, only the numbers that have significance (derived from measurement) are written.

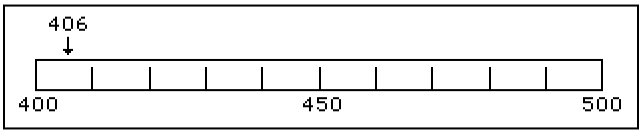
Rule 1: Non-zero digits are always significant.

Hopefully, this rule seems rather obvious. If you measure something and the device you use (ruler, thermometer, triple-beam balance, etc.) returns a number to you, then you have made a measurement decision and that ACT of measuring gives significance to that particular numeral (or digit) in the overall value you obtain.

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:

0.005**00**

0.0304**0**

Here are two more examples where the significant zeros are in boldface:

2.3**0** x 10^{-5}

4.5**00** x 10^{12}

What Zeros are Not Discussed Above

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

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

0.**00**500

0.**0**3040

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 x 10^{-3} and 3.040 x 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 significnt 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 2.0×10^2 is used. If it has three, then 2.00×10^2 is used. If it had four, then 200.0 is sufficient. See rule #2 above.

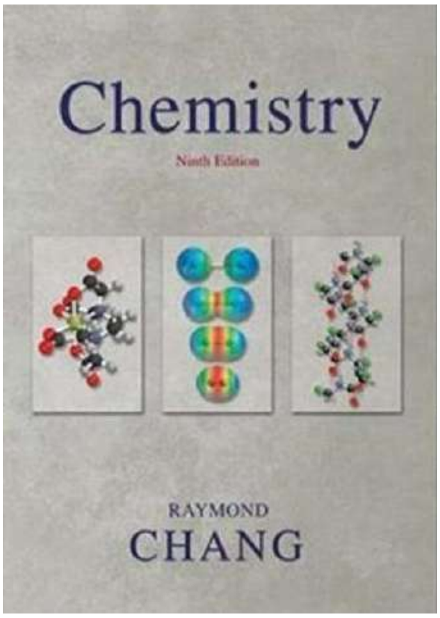
How will you know how many significant figures are in a number like 200? In a problem like below, divorced of all scientific context, you will be told. If you were doing an experiment, the context of the experiment and its measuring devices would tell you how many significant figures to report to people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

Zero Type #4: leading zeros in a whole number.

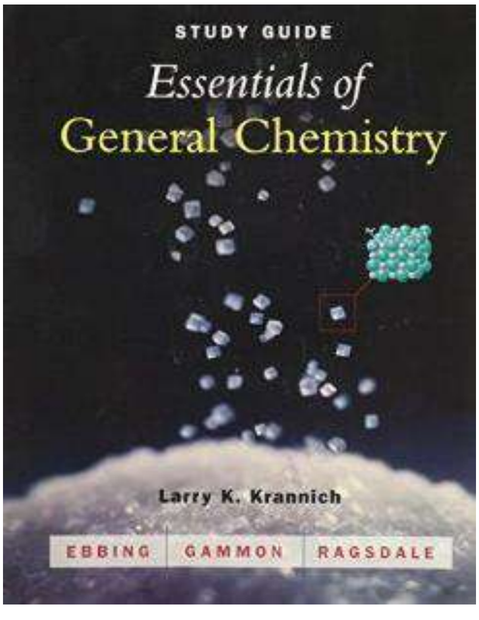
00250 has two significant figures. 005.00×10^{-4} has three.

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.

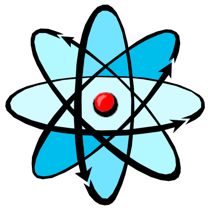


2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 2

Atoms, Molecules and Ions



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

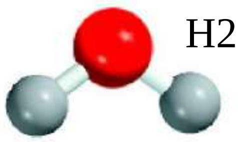
2.6 Chemical Formula

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 element.
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.



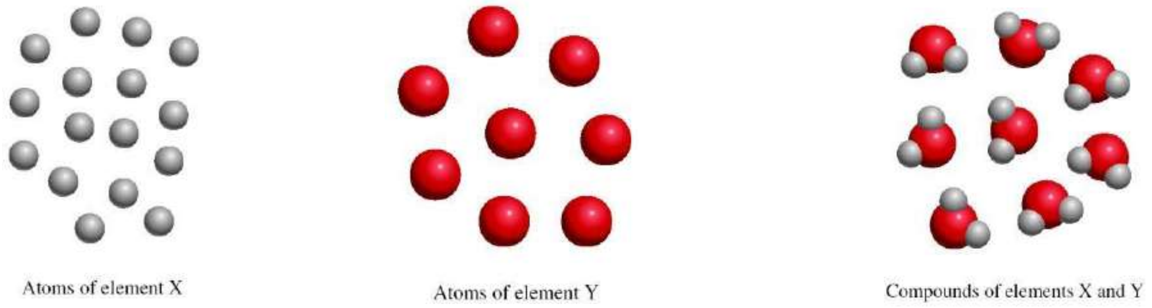
H2O

Law of Definite Proportions

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

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.



$$16\ X \quad + \quad 8\ Y \longrightarrow 8\ X_2Y$$

Law of Conservation of Mass

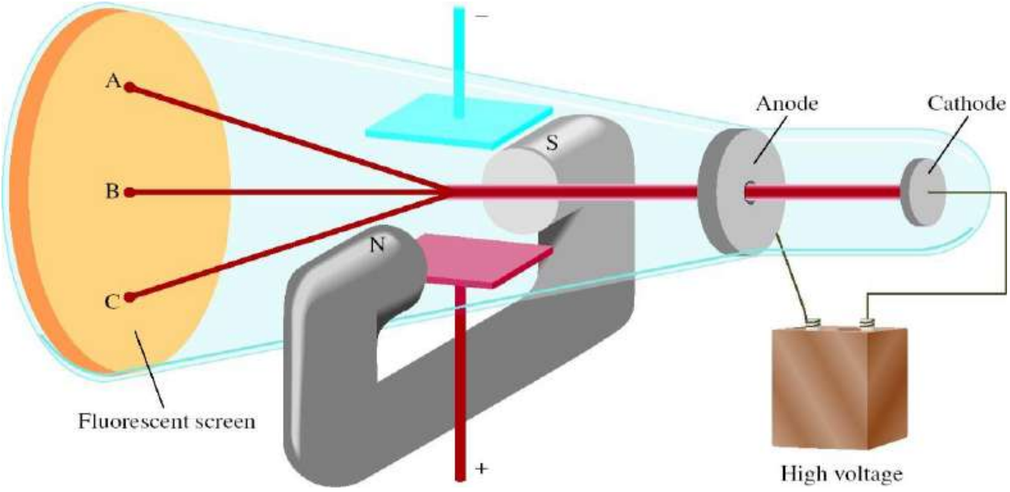
- Matter is neither created nor destroyed

The Modern View of Atomic Structure

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

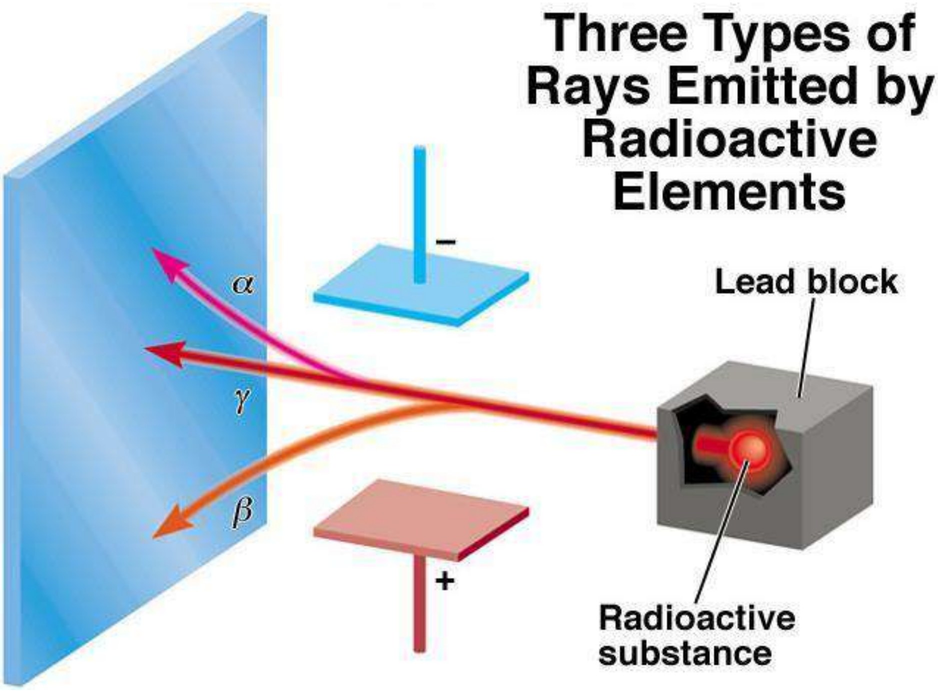
Three **subatomic particles -** electrons , protons, and neutrons.

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 x 10^{-28} g).



(Uranium

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

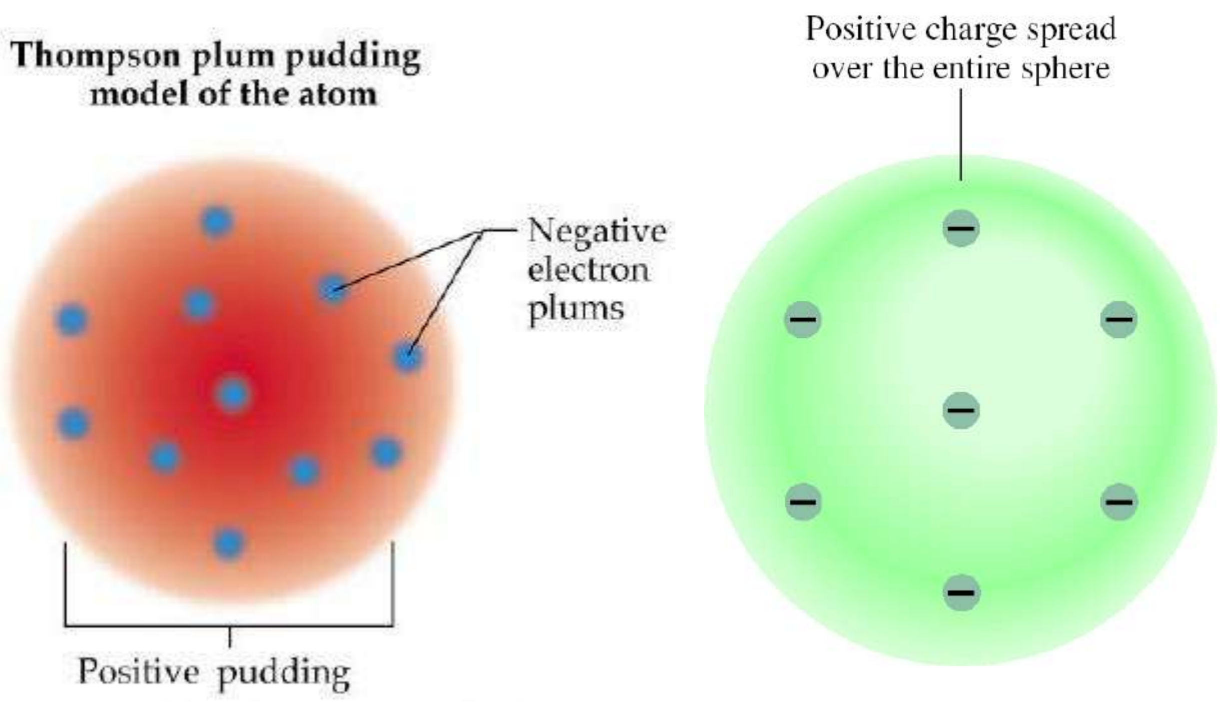
(i) **Alpha (α) rays** .. positively charged particles (α) particles .. deflected by positively charged plate

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

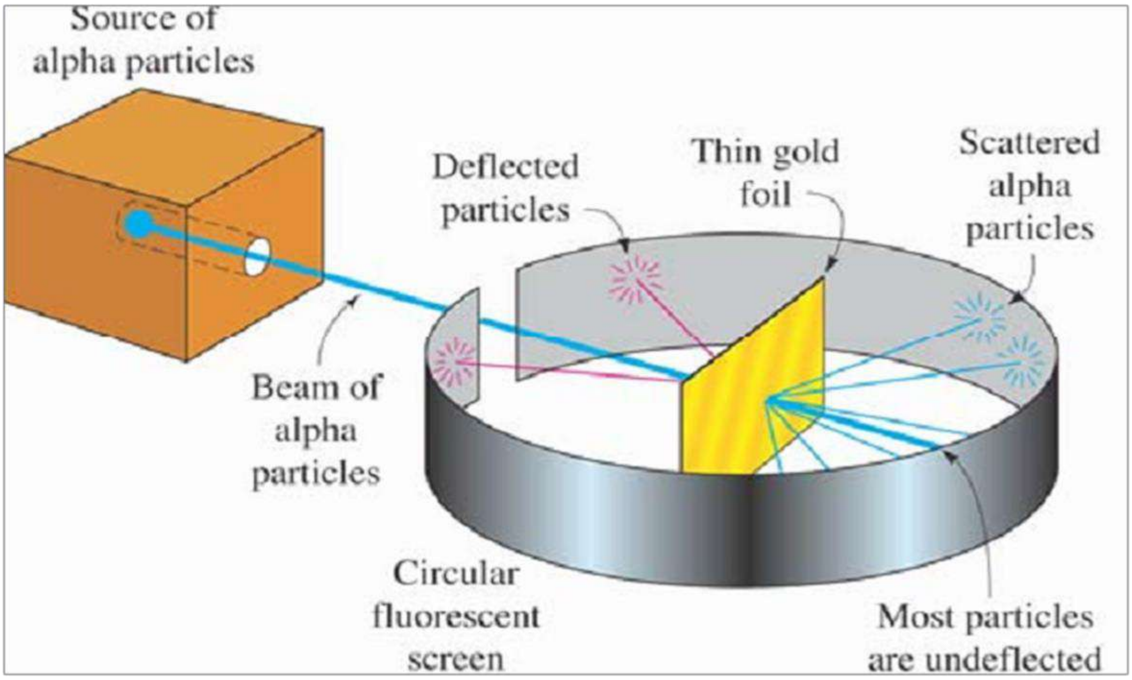
(iii) **Gamma (γ) rays ..** high-energy rays .. no charge and are not affected by an external field.

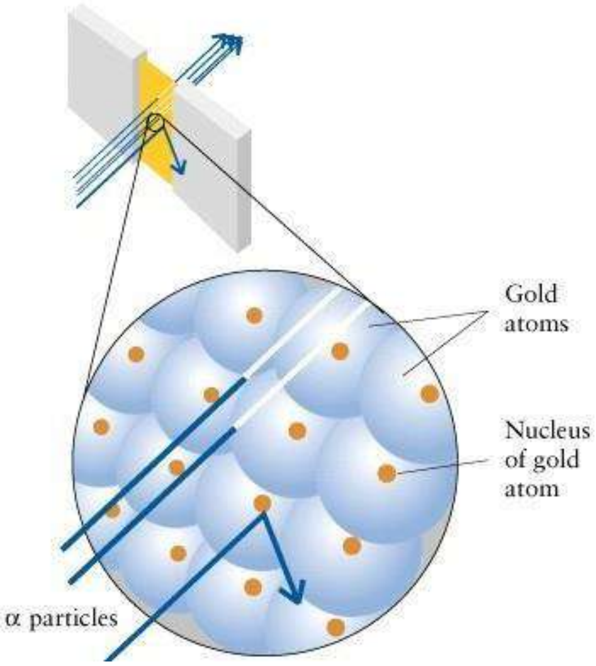
Thomson's Model

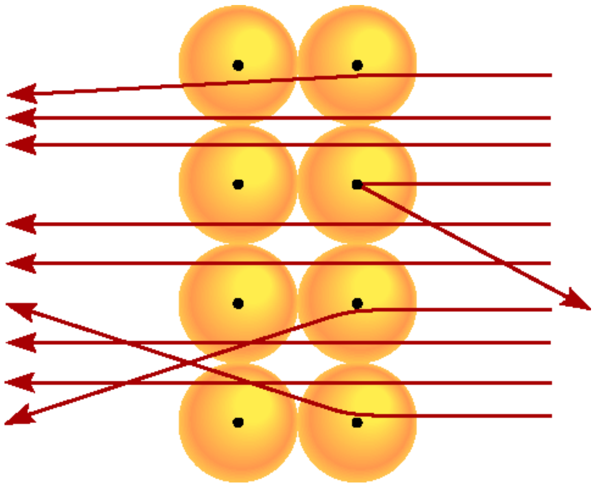
– a spherical atom composed of diffuse, positively charge matter, in which e- embedded like "**raisin in a plum pudding**".



Rutherford's gold foil α-scattering experiment

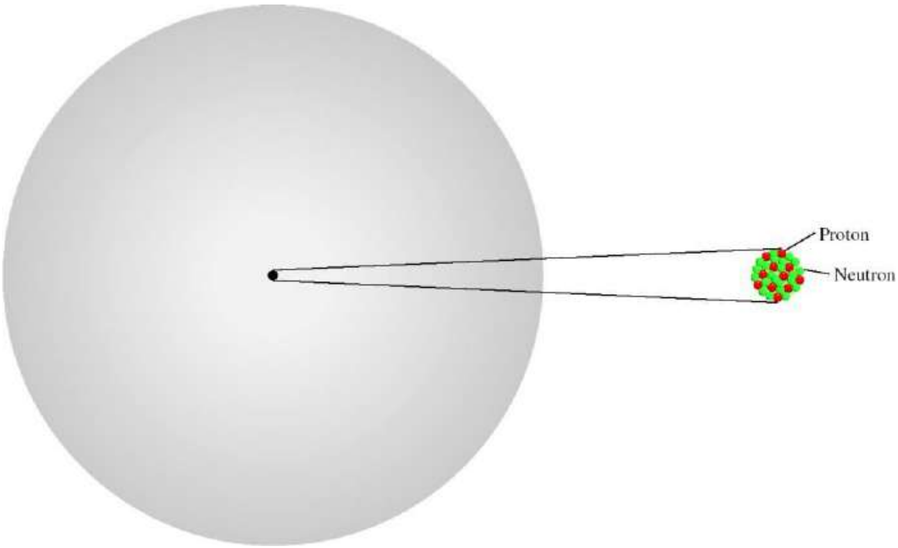






Rutherford's Model of the Atom

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^- (1.67 x 10^{-24} g)



atomic radius ~ 100 pm = 1 x 10-10 m
nuclear radius ~ 5 x 10-3 pm = 5 x 10-15 m

Chadwick's Experiment (1932)

0n **2n**

H atoms - 1 p; He atoms - 2 p

mass He/mass H should = 2

measured mass He/mass H = 4

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

TABLE 2.1	Mass and Charge of Subatomic Particles		
		Charge	
Particle	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^-

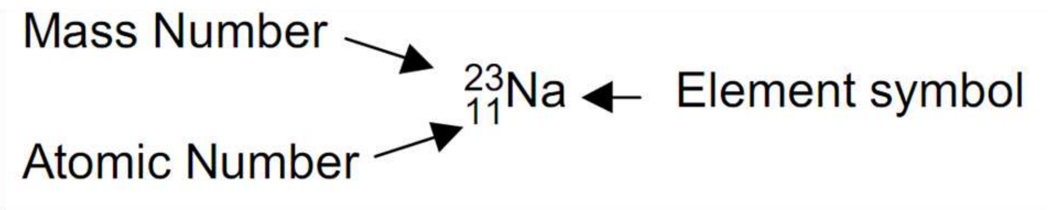
Atomic number, Mass number and Isotopes

Atomic number (Z) = number of protons in nucleus

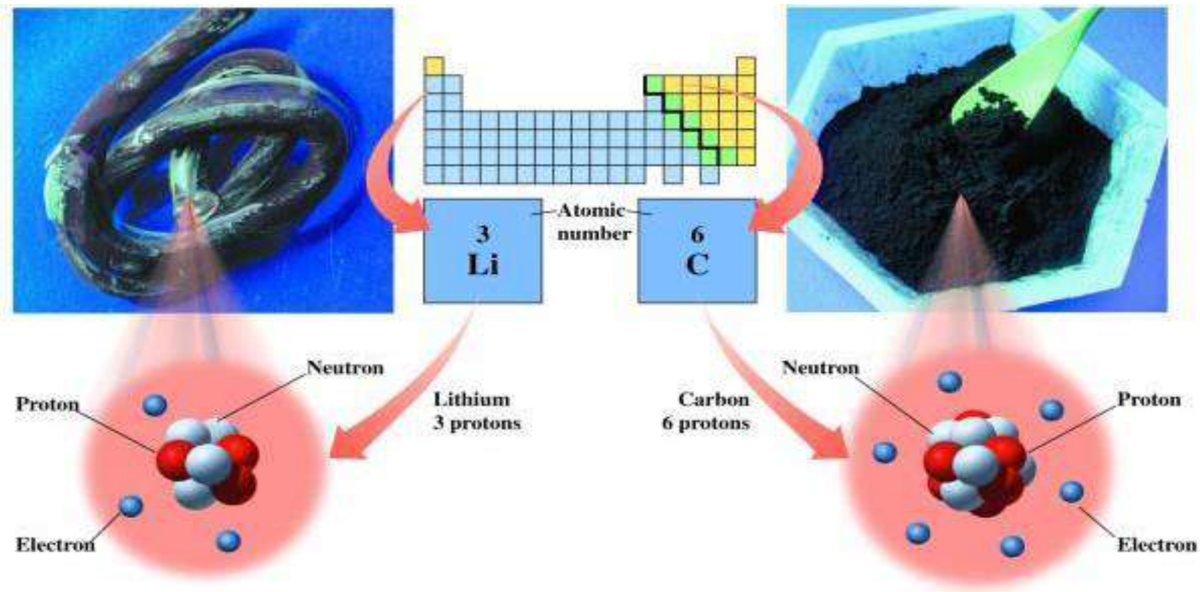
Mass number (A) = number of protons + number of neutrons

= atomic number (Z) + number of neutrons

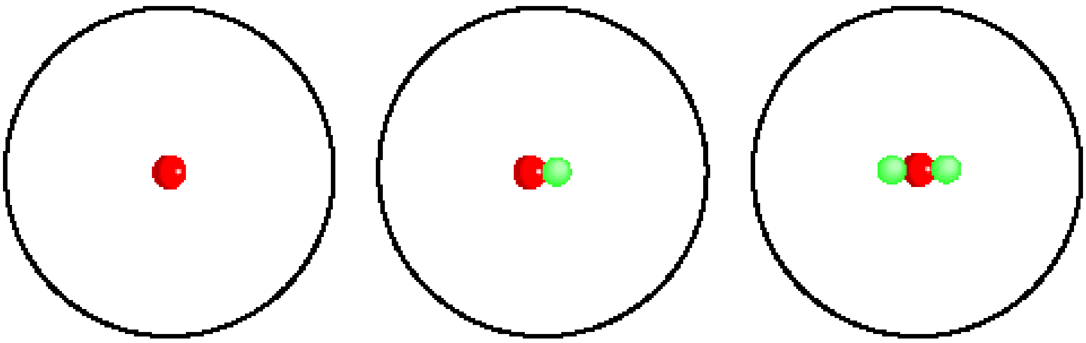
Isotopes are atoms of the same element (X) that have the same atomic number but different mass numbers



$^{1}_{1}H$ $^{2}_{1}H$ (D) $^{3}_{1}H$ (T) $^{235}_{92}U$ $^{238}_{92}U$



The Isotopes of Hydrogen



$^{1}_{1}H$ $^{2}_{1}H$ $^{3}_{1}H$

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 $^{14}_{6}C$?

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

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

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

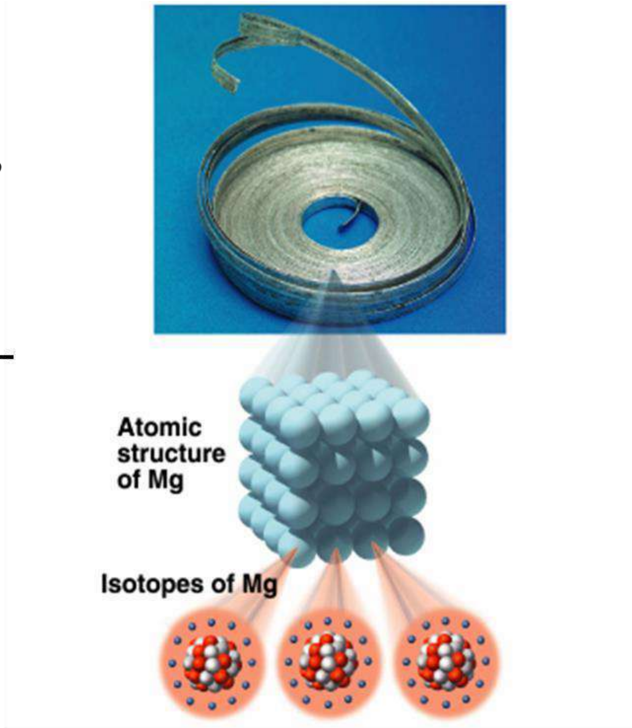
Naturally occurring carbon consists of three isotopes, ^{12}C, ^{13}C, and ^{14}C. State the number of protons, neutrons, and electrons in each of the following.

	$^{12}_{6}C$	$^{13}_{6}C$	$^{14}_{6}C$
Proton	**6**	**6**	**6**
Neutron	**6**	**7**	**8**
Electron	**6**	**6**	**6**

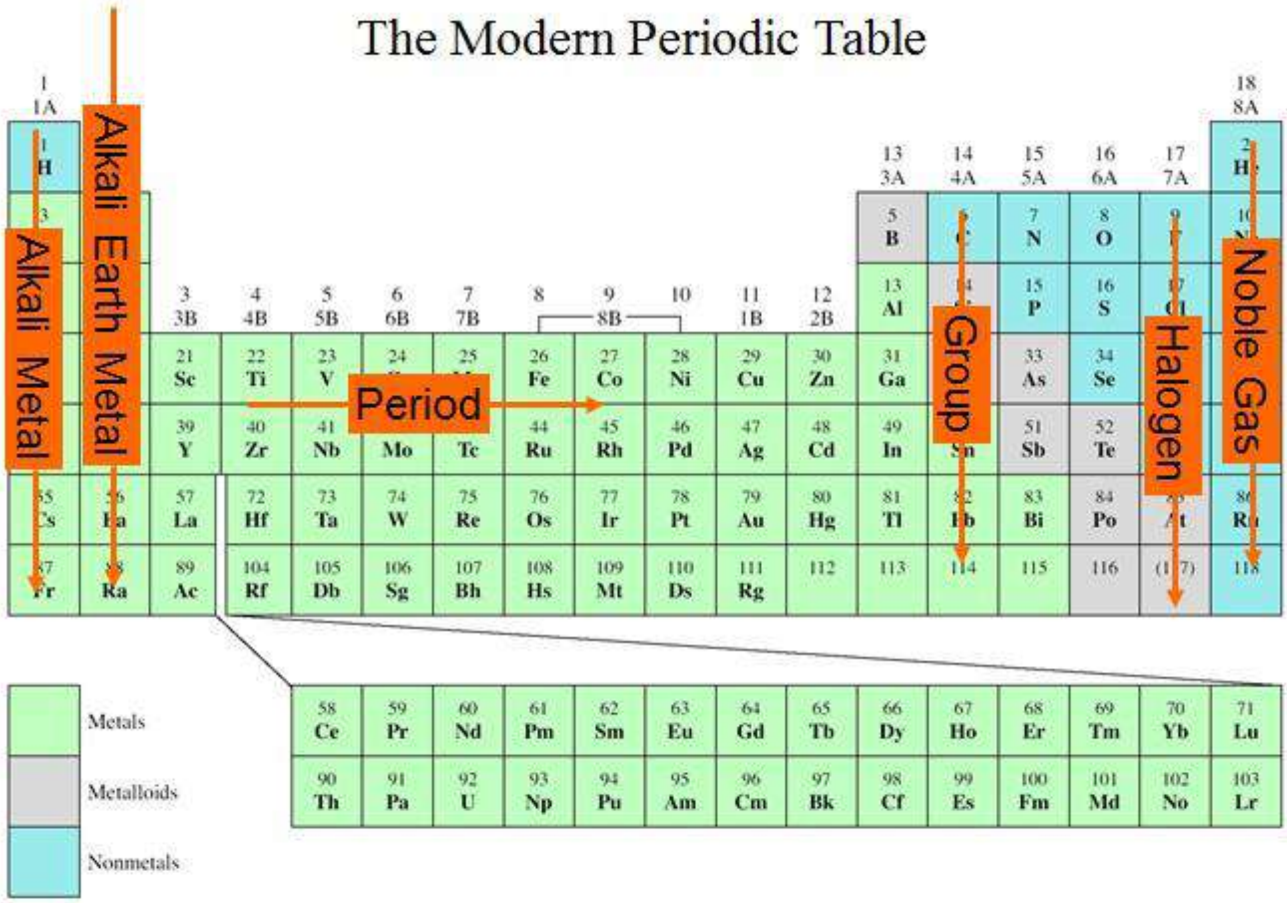
In naturally occurring magnesium, there are three isotopes.

Isotopes of Mg

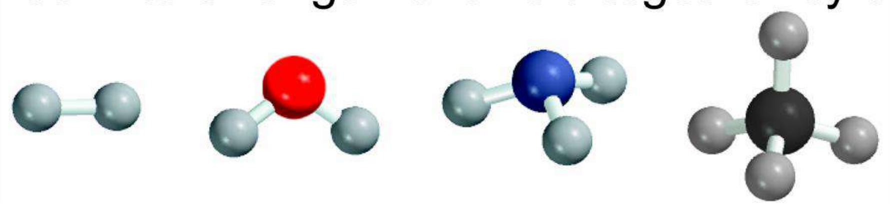
Atomic symbol	$^{24}_{12}Mg$	$^{25}_{12}Mg$	$^{26}_{12}Mg$
Number of protons	12	12	12
Number of electrons	12	12	12
Mass number	24	25	26
Number of neutrons	12	13	14



$^{24}_{12}Mg$ $^{25}_{12}Mg$ $^{26}_{12}Mg$



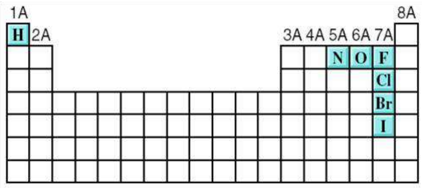
A ***molecule*** is an aggregate of two or more atoms in a definite arrangement held together by chemical forces



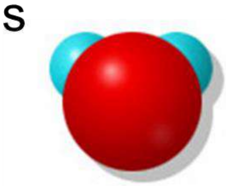
N_2
Nitrogen gas - a homonuclear molecule

A ***diatomic molecule*** contains only two atoms

H_2, N_2, O_2, Br_2, HCl, CO



diatomic elements



H_2O
Water - a heteronuclear molecule

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

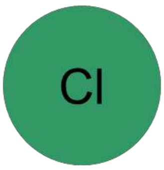
If a neutral atom **loses** one or more electrons it becomes a cation.

11 protons
11 electrons

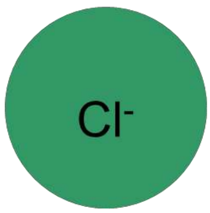
11 protons
10 electrons

anion – ion with a negative charge

If a neutral atom **gains** one or more electrons it becomes an anion.



17 protons
17 electrons



17 protons
18 electrons

A ***monatomic ion*** contains only one atom

$$Na^{+}, Cl^{-}, Ca^{2+}, O^{2-}, Al^{3+}, N^{3-}$$

A ***polyatomic ion*** contains more than one atom

$$OH^{-}, CN^{-}, NH_4^{+}, CO_3^{2-}, HCO_3^{-}, SO_4^{2-}, PO_4^{3-}, NO_3^{-}, NO_2^{-}$$

The names of common polyatomic anions

- end in *ate.*

  NO_3^{-} nitr**ate** PO_4^{3-} phosph**ate**

- with **one oxygen less** end in *ite*.

  NO_2^{-} nitr**ite** PO_3^{3-} phosph**ite**

- with hydrogen attached use the prefix *hydrogen* (or *bi).*

  HCO_3^{-} **hydrogen** carbonate (**bi**carbonate)

  HSO_3^{-} **hydrogen** sulfite (**bi**sulfite)

Common Ions Shown on the Periodic Table

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
Li^+													C^{4-}	N^{3-}	O^{2-}	F^-	
Na^+	Mg^{2+}											Al^{3+}		P^{3-}	S^{2-}	Cl^-	
K^+	Ca^{2+}				Cr^{2+} Cr^{3+}	Mn^{2+} Mn^{3+}	Fe^{2+} Fe^{3+}	Co^{2+} Co^{3+}	Ni^{2+} Ni^{3+}	Cu^+ Cu^{2+}	Zn^{2+}				Se^{2-}	Br^-	
Rb^+	Sr^{2+}									Ag^+	Cd^{2+}		Sn^{2+} Sn^{4+}		Te^{2-}	I^-	
Cs^+	Ba^{2+}									Au^+ Au^{3+}	Hg_2^{2+} Hg^{2+}		Pb^{2+} Pb^{4+}				

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

13 protons, 10 (13 – 3) electrons

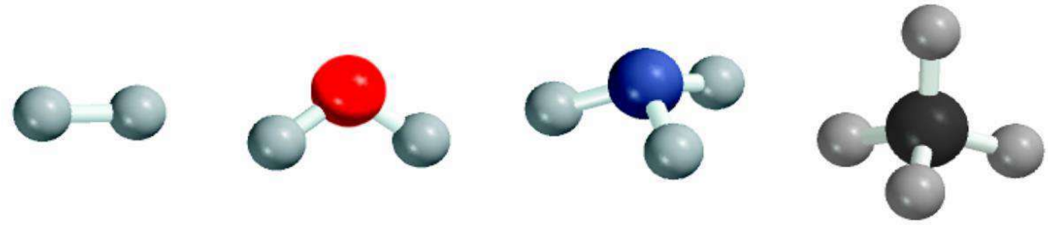
How many protons and electrons are in $^{78}_{34}Se^{2-}$?

34 protons, 36 (34 + 2) electrons

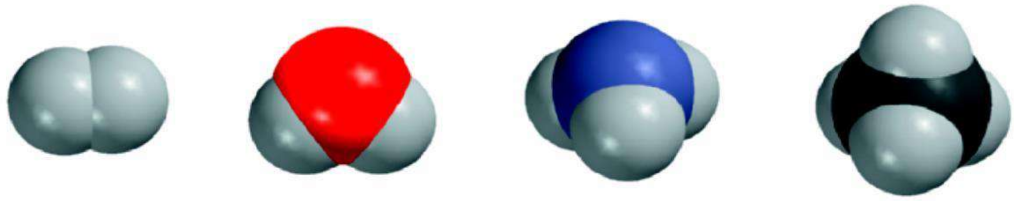
Formulas and Models

	Hydrogen	Water	Ammonia	Methane
Molecular formula	H_2	H_2O	NH_3	CH_4
Structural formula	H—H	H—O—H	H—N—H H	H H—C—H H

Ball-and-stick model



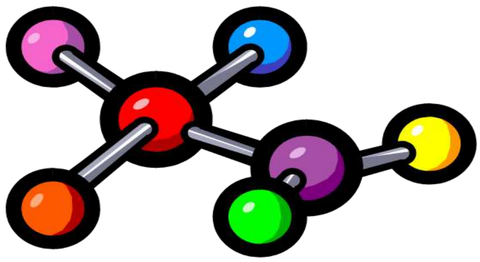
Space-filling model



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

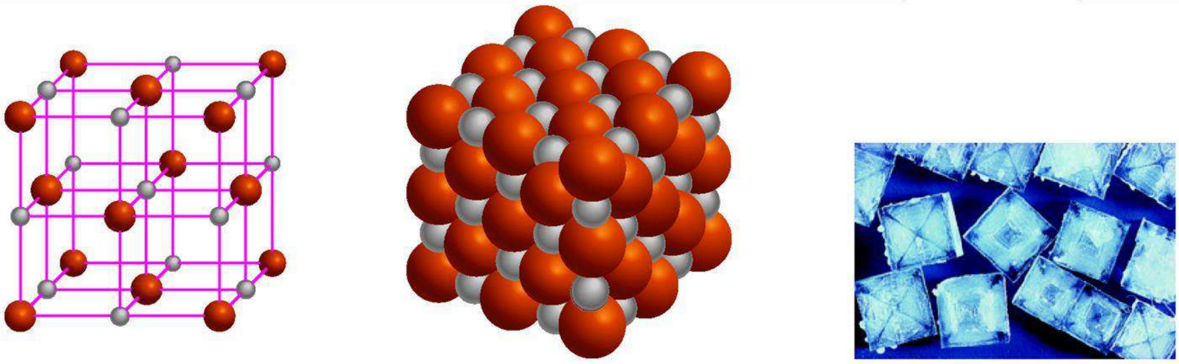
molecular	**empirical**
H_2O	H_2O
$C_6H_{12}O_6$	CH_2O
O_3	O
N_2H_4	NH_2

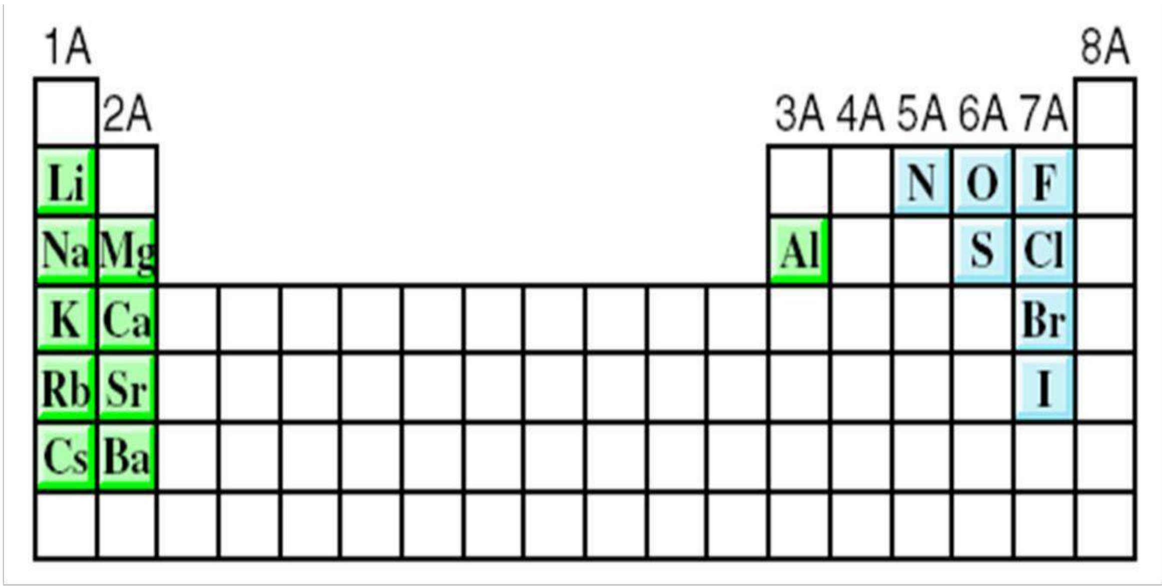


ionic compounds consist of a combination of cations and an anions

- 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

$2 \times +3 = +6$ $3 \times -2 = -6$

Al_2O_3

Al^{3+} O^{2-}

$1 \times +2 = +2$ $2 \times -1 = -2$

$CaBr_2$

Ca^{2+} Br^{-}

$1 \times +2 = +2$ $1 \times -2 = -2$

Na_2CO_3

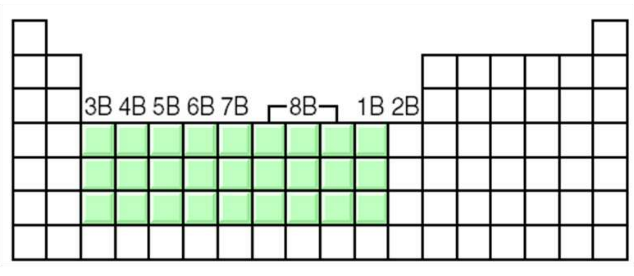
Na^{+} CO_3^{2-}

Chemical Nomenclature

- **Ionic Compounds**
  - Most are binary compounds, some are ternary compounds
  - Often a metal + nonmetal
  - Anion (nonmetal), add “ide” to element name

$BaCl_2$	barium chloride
K_2O	potassium oxide
$Mg(OH)_2$	magnesium hydroxide
KNO_3	potassium nitrate

- Transition metal ionic compounds
  - indicate charge on metal with **Roman numerals**



+1	+2	+3	+4	+5
(I)	(II)	(III)	(IV)	(V)

$FeCl_2$	2 Cl^- -2 so Fe is +2	iron(II) chloride
$FeCl_3$	3 Cl^- -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 Ions	Name of Ion
Chromium	Cr^{2+}	chromium(II)
	Cr^{3+}	chromium(III)
Copper	Cu^{+}	copper(I)
	Cu^{2+}	copper(II)
Gold	Au^{+}	gold(I)
	Au^{3+}	gold(III)
Iron	Fe^{2+}	iron(II)
	Fe^{3+}	iron(III)
Lead	Pb^{2+}	lead(II)
	Pb^{4+}	lead(IV)

$FeCl_2$	iron(II) chloride
$FeCl_3$	iron(III) chloride
Cu_2S	copper(I) sulfide
$CuCl_2$	copper(II) chloride
$SnCl_2$	tin(II) chloride
$PbBr_4$	lead(IV) bromide

TABLE 2.2 The "-ide" Nomenclature of Some Common Monatomic Anions According to Their Positions in the Periodic Table

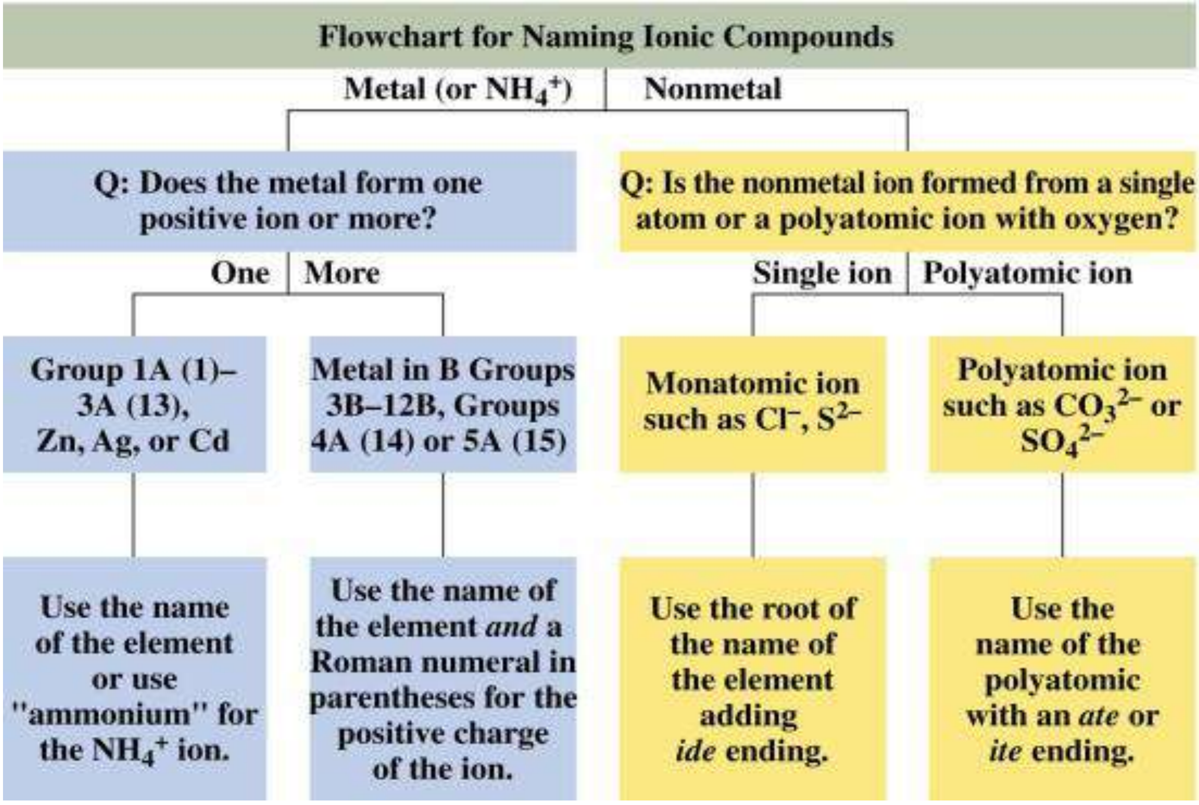
Group 4A	Group 5A	Group 6A	Group 7A
C carbide (C^{4-})*	N nitride (N^{3-})	O oxide (O^{2-})	F fluoride (F^{-})
Si silicide (Si^{4-})	P phosphide (P^{3-})	S sulfide (S^{2-})	Cl chloride (Cl^{-})
		Se selenide (Se^{2-})	Br bromide (Br^{-})
		Te telluride (Te^{2-})	I iodide (I^{-})

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

TABLE 2.3 Names and Formulas of Some Common Inorganic Cations and Anions

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 ($H_2PO_4^-$)
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^-)

*Mercury(I) exists as a pair as shown.



- **Molecular compounds**
  - Nonmetals or nonmetals + metalloids
  - Common names
    - H_2O, NH_3, CH_4,
  - 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*

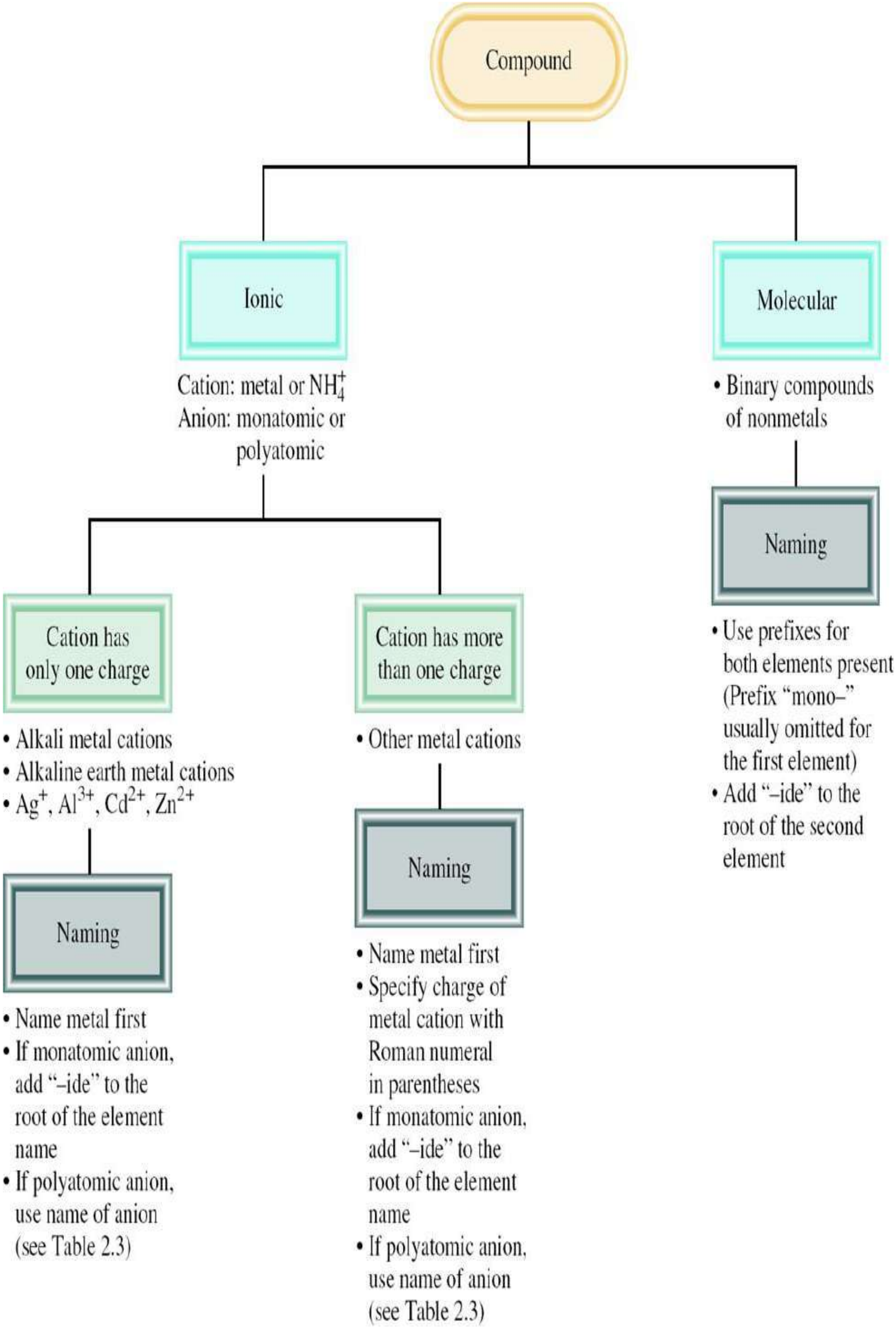
TABLE 2.4

Greek Prefixes Used in Naming Molecular Compounds

Prefix	Meaning
mono-	1
di-	2
tri-	3
tetra-	4
penta-	5
hexa-	6
hepta-	7
octa-	8
nona-	9
deca-	10

Molecular Compounds

HI	hydrogen iodide
NF_3	nitrogen trifluoride
SO_2	sulfur dioxide
N_2Cl_4	dinitrogen tetrachloride
NO_2	nitrogen dioxide
N_2O	dinitrogen monoxide



Compound
Ionic
Cation: metal or NH_4^+
Anion: monatomic or polyatomic
Molecular
• Binary compounds of nonmetals
Cation has only one charge
• Alkali metal cations
• Alkaline earth metal cations
• Ag^+, Al^{3+}, Cd^{2+}, Zn^{2+}
Naming
• Name metal first
• If monatomic anion, add "–ide" to the root of the element name
• If polyatomic anion, use name of anion (see Table 2.3)
Cation has more than one charge
• Other metal cations
Naming
• Name metal first
• Specify charge of metal cation with Roman numeral in parentheses
• If monatomic anion, add "–ide" to the root of the element name
• If polyatomic anion, use name of anion (see Table 2.3)
Naming
• Use prefixes for both elements present (Prefix "mono–" usually omitted for the first element)
• Add "–ide" to the root of the second element

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
- Dissolved in water (H_3O^+ and Cl^-), hydrochloric acid

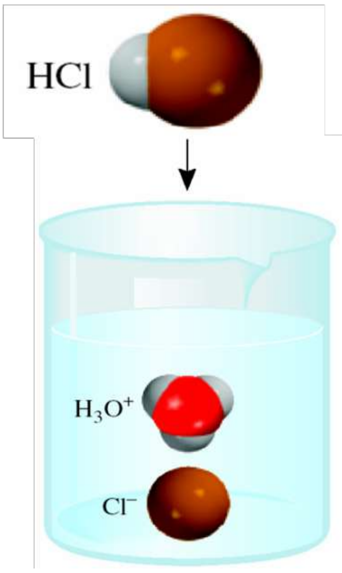


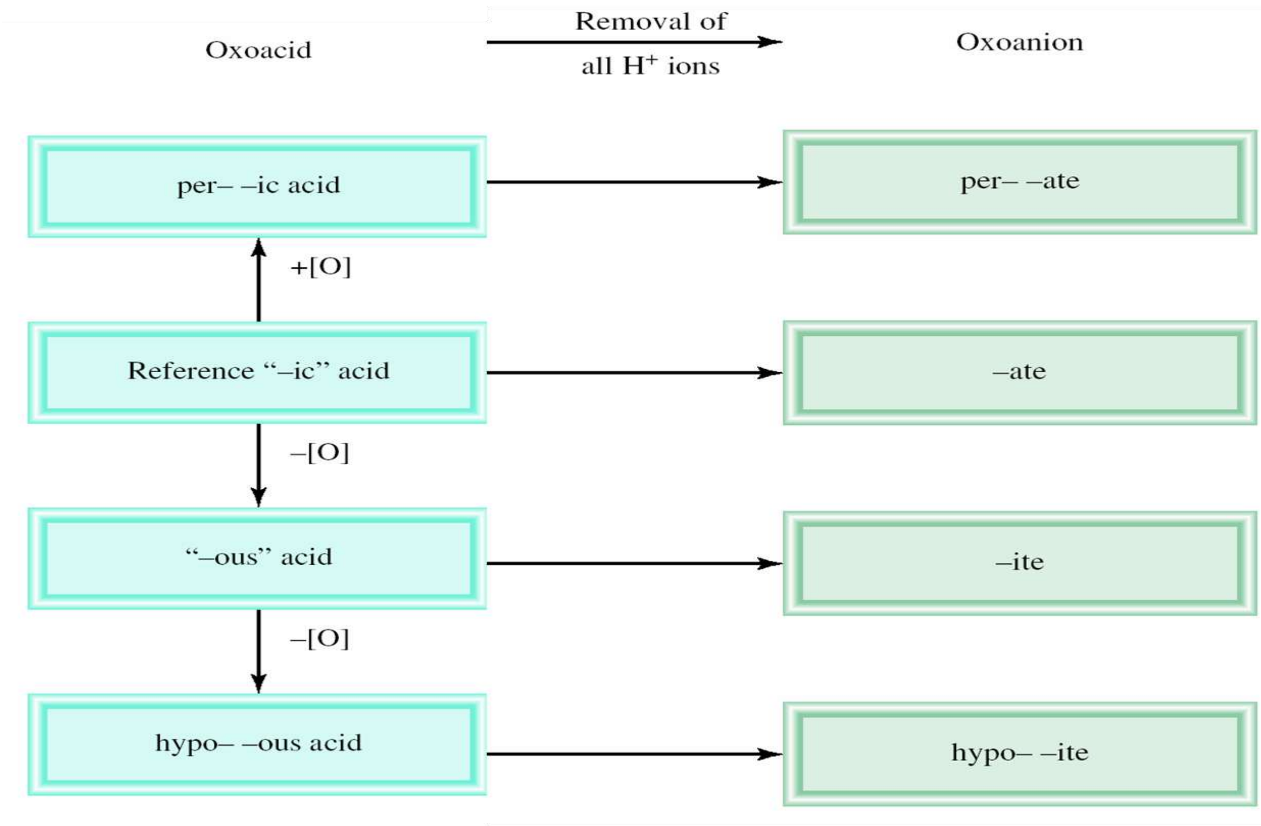
TABLE 2.5 Some Simple Acids

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)

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

HNO_3	nitric acid
HNO_2	nitrous acid
H_2SO_4	sulfuric acid
H_2SO_3	sulfurous acid
H_2CO_3	carbonic acid
H_3PO_4	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:
   - $H_2PO_4^-$ dihydrogen phosphate
   - HPO_4^{2-} hydrogen phosphate
   - PO_4^{3-} 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 hydroxide
KOH	potassium hydroxide
$Ba(OH)_2$	barium hydroxide

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

$BaCl_2 \cdot 2H_2O$	barium chloride dihydrate
$LiCl \cdot H_2O$	lithium chloride monohydrate
$MgSO_4 \cdot 7H_2O$	magnesium sulfate heptahydrate
$Sr(NO_3)_2 \cdot 4H_2O$	strontium nitrate tetrahydrate

$CuSO_4 \cdot 5H_2O$ →

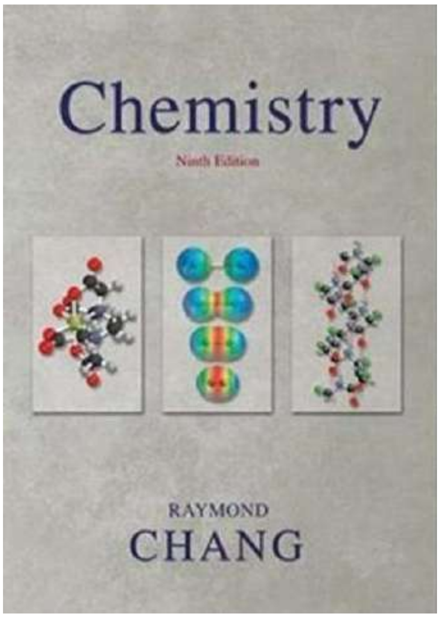
← $CuSO_4$

TABLE 2.7 Common and Systematic Names of Some Compounds

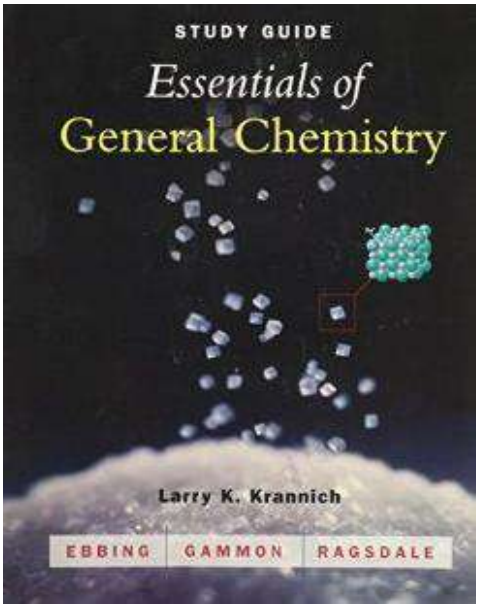
Formula	Common Name	Systematic Name
H_2O	Water	Dihydrogen monoxide
NH_3	Ammonia	Trihydrogen nitride
CO_2	Dry ice	Solid carbon dioxide
NaCl	Table salt	Sodium chloride
N_2O	Laughing gas	Dinitrogen monoxide
$CaCO_3$	Marble, chalk, limestone	Calcium carbonate
CaO	Quicklime	Calcium oxide
$Ca(OH)_2$	Slaked 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

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.

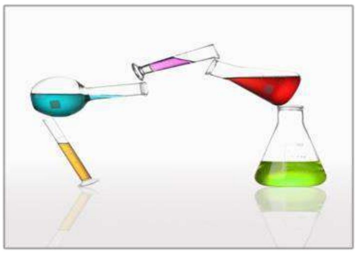


2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 3

Mass Relationships in Chemical Reactions



3.1 Atomic Mass

3.2 Molar mass and Avogadro's Number

3.3 Molecular Mass

3.4 Percent Composition of Compounds

3.5 Chemical Reactions and Chemical Equations

3.6 Amounts of Reactants and Products

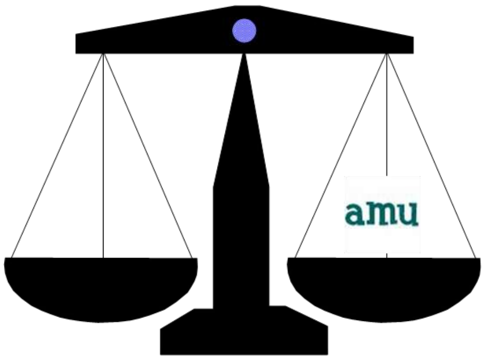
3.7 Limiting Reagents

3.8 Reaction Yield

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 one-twelfth of the mass of one carbon-12 atom.



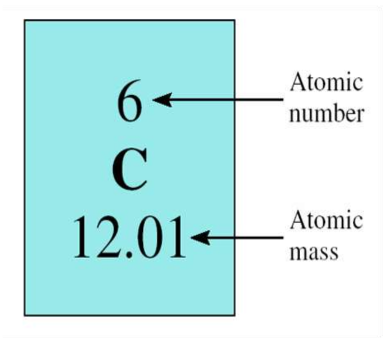
By definition:
1 atom ^{12}C "weighs" 12 amu

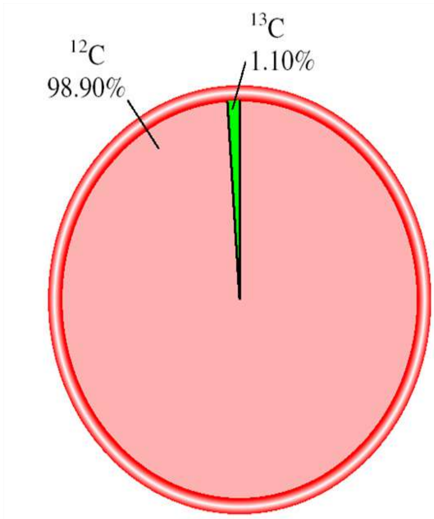
On this scale

^{1}H = 1.00794 amu

^{16}O = 15.9994 amu

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

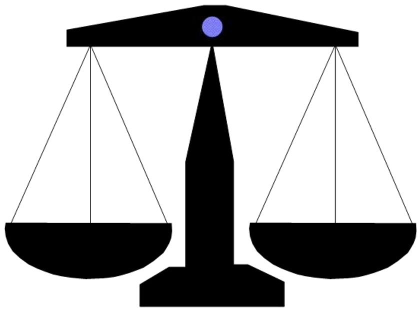




Natural lithium is:

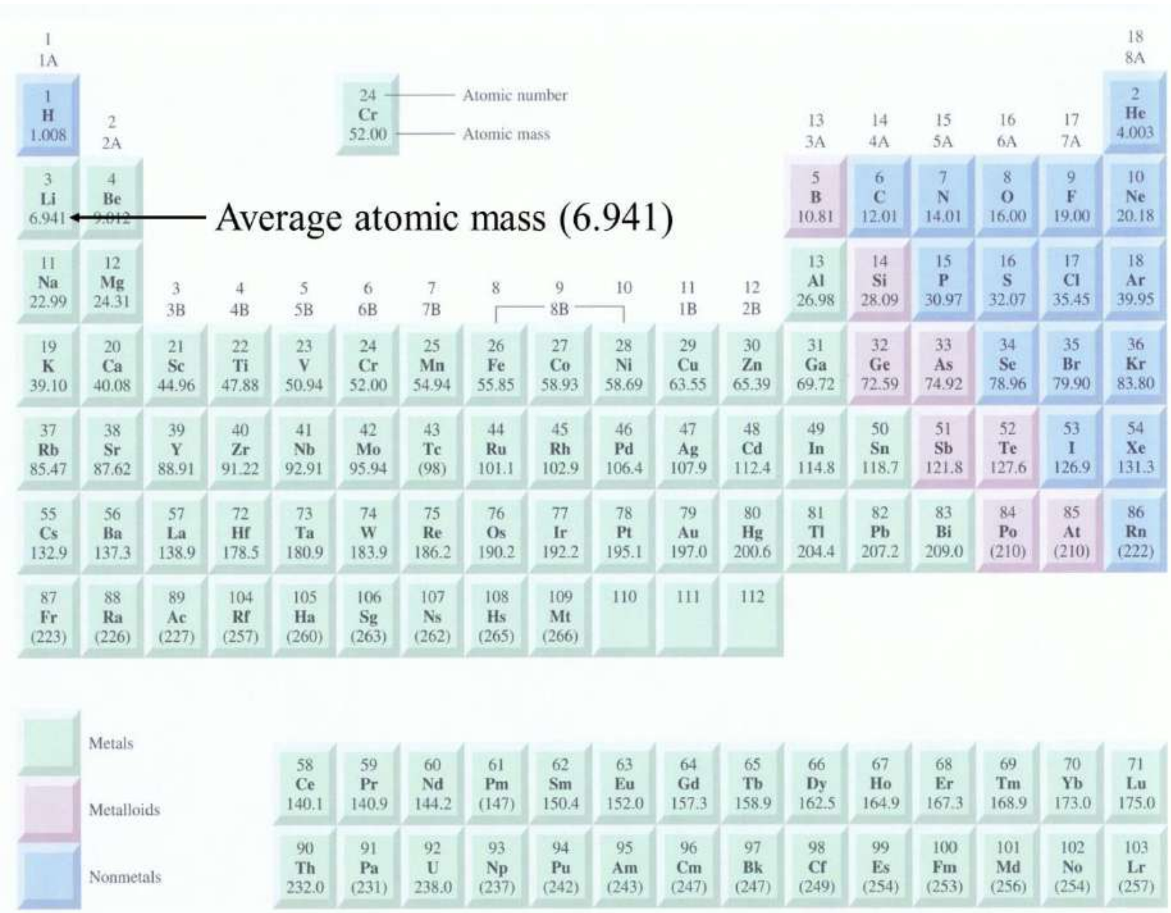
7.42% ^{6}Li (6.015 amu)

92.58% ^{7}Li (7.016 amu)

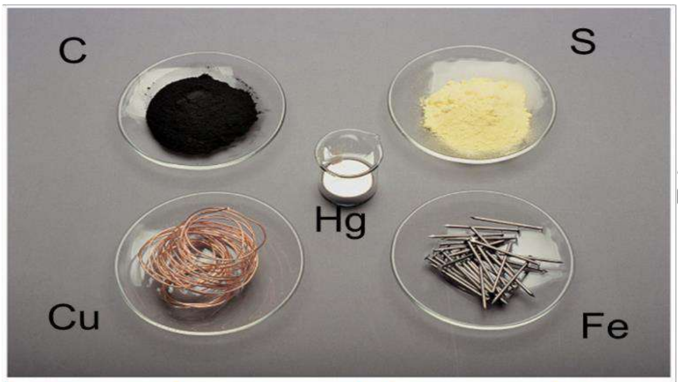


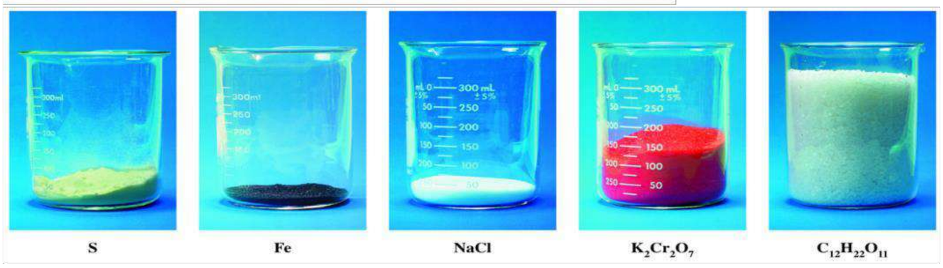
Average atomic mass of lithium:

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



One-Mole Quantities





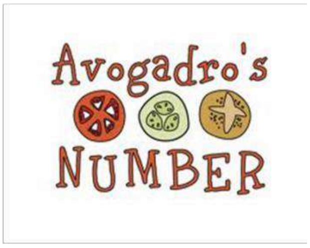
32.1 g 55.9 g 58.5 g 294.2 g 342.2 g

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.

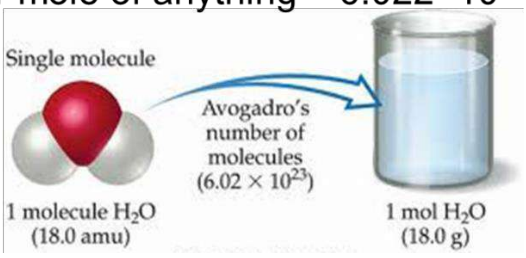
$$1 \text{ mol} = N_A = 6.0221367 \times 10^{23}$$

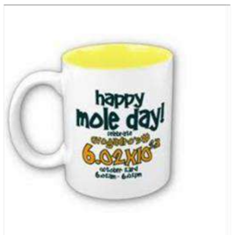
Avogadro's number (N_A)

1 mole	Number of Atoms
1 mole C	= 6.02×10^{23} C atoms
1 mole Na^+	= 6.02×10^{23} Na^+ ions
1 mole H_2O	= 6.02×10^{23} H_2O molecules

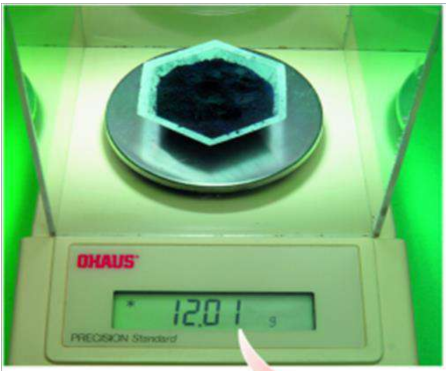


1 mole of anything = 6.022×10^{23} units of that thing





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



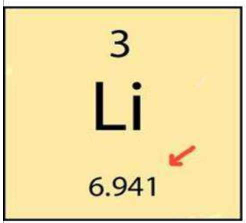
1 mol ^{12}C atoms = 6.022×10^{23} atoms

1 ^{12}C atom = 12.00 amu

1 amu = 1.661×10^{-24} g

1 mol ^{12}C atoms = 12.00 g ^{12}C

1 mol lithium atoms = 6.941 g of Li



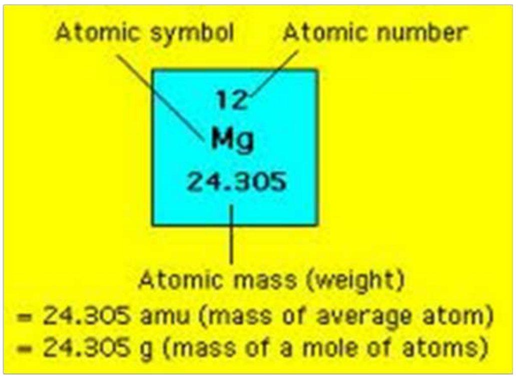
6.022×10^{23} atoms C

1 mol C atoms

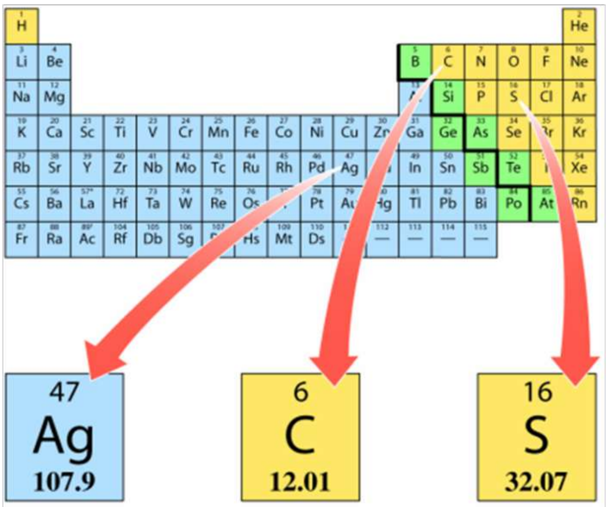
12.01 g C atoms

For any element
atomic mass (amu) = molar mass (grams)

Molar Mass from Periodic Table



Molar mass is the atomic mass expressed in grams.

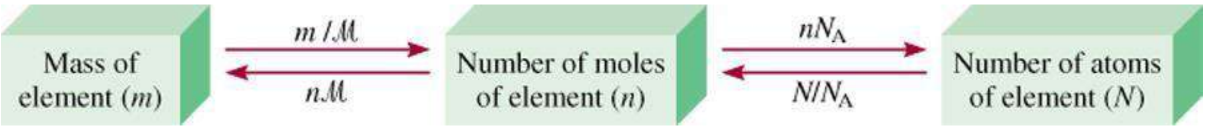


1 mole Ag = 107.9 g

1 mole C = 12.01 g

1 mole S = 32.07 g

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



M = molar mass in g/mol

N_A = Avogadro's number

Do You Understand Molar Mass?

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

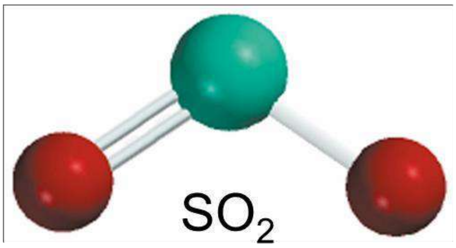
1 mol of K = 39.10 g of K

1 mol of K = 6.022×10^{23} atoms of K

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

8.49×10^{21} atoms of K

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

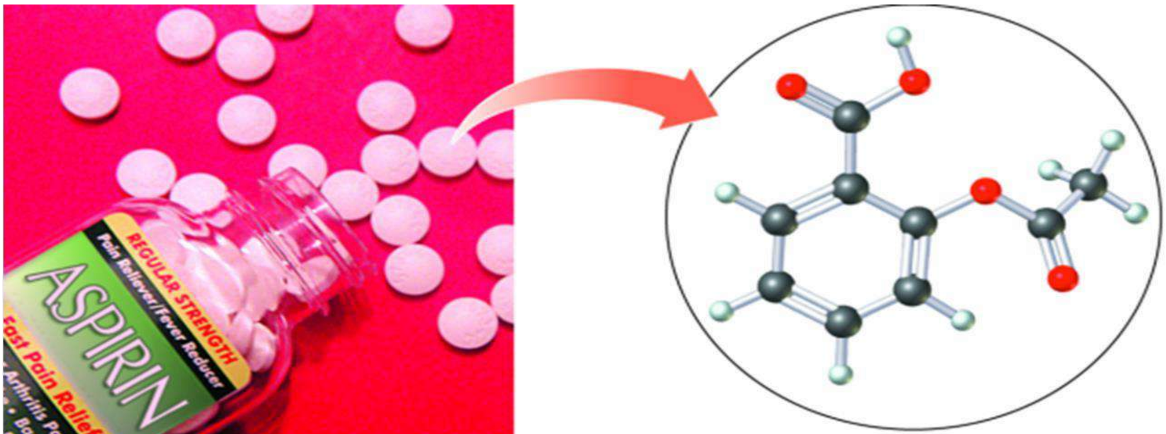


1S	32.07 amu
2O	+ 2 x 16.00 amu
SO_2	64.07 amu

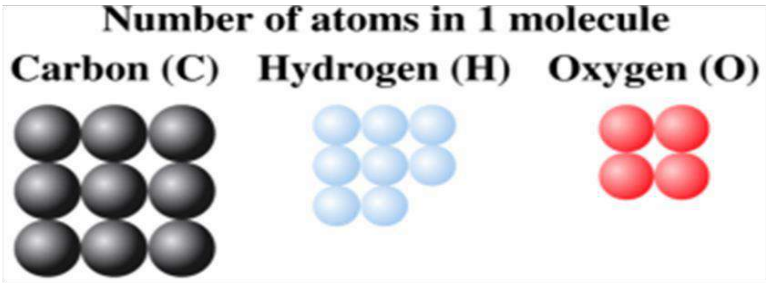
> For any molecule
>
> molecular mass in amu = molar mass in grams

1 molecule of SO_2 weighs 64.07 amu

1 mole of SO_2 weighs 64.07 g



Aspirin $C_9H_8O_4$



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 g / 60.095 g/mol = 1.21 mol

1 mol C_3H_8O molecules contains 8 mol H atoms

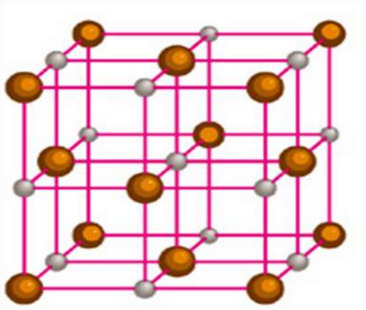
1 mol of H atoms is 6.022×10^{23} H atoms

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

5.82×10^{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	+ 35.45 amu
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 $Ca_3(PO_4)_2$?

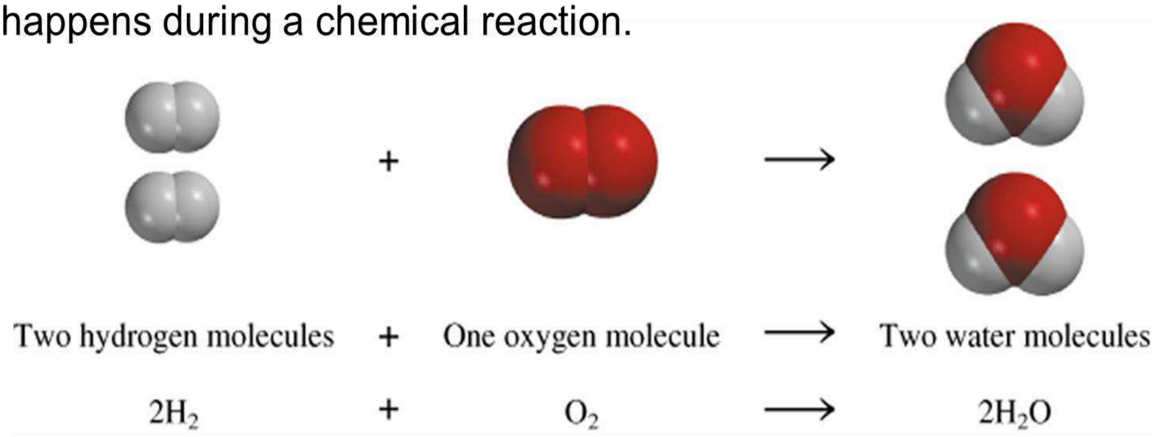
1 formula unit of $Ca_3(PO_4)_2$

3 Ca		3 x 40.08 g/mol
2 P		2 x 30.97 g/mol
8 O	+	8 x 16.00 g/mol
		310.18 g/mol

Units of grams per mole are the most practical for chemical calculations!

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.

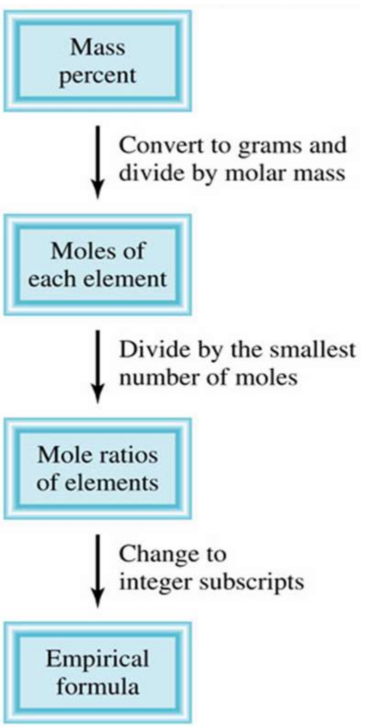


reactants ⟶ products

In a **balanced chemical reaction**

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

Percent Composition and Empirical Formulas



$n_K = 0.6330,\ n_{Mn} = 0.6329,\ n_O = 2.532$

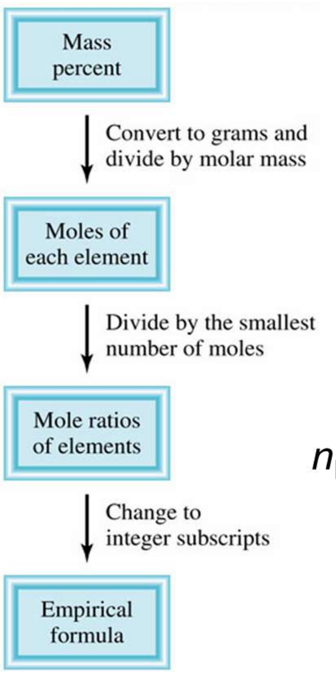
$$K : \frac{0.6330}{0.6329} \approx 1.0$$

$$Mn : \frac{0.6329}{0.6329} = 1.0$$

$$O : \frac{2.532}{0.6329} \approx 4.0$$

$KMnO_4$

Percent Composition and Empirical Formulas



Determine the empirical formula of a compound that has the following percent composition by mass:
K 24.75%, Mn 34.77%, O 40.51% percent.

$$n_K = 24.75\ \cancel{g\ K} \times \frac{1\ mol\ K}{39.10\ \cancel{g\ K}} = 0.6330\ mol\ K$$

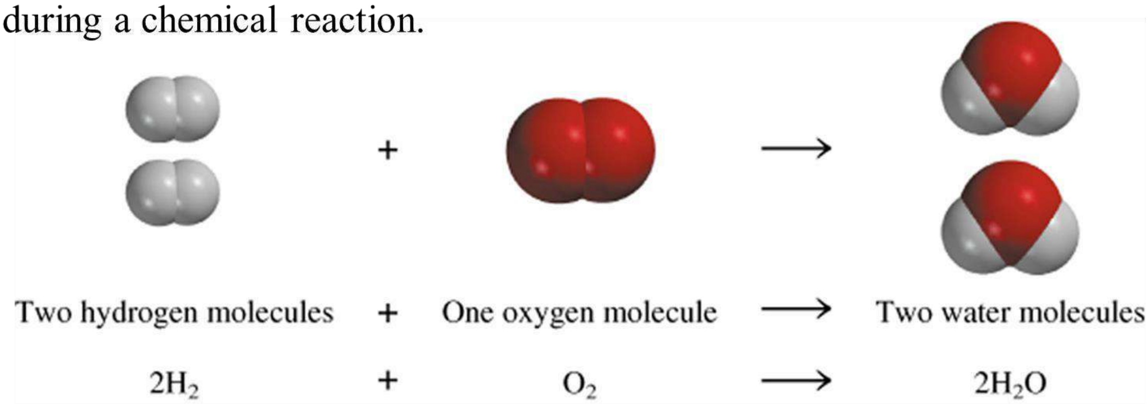
$$n_{Mn} = 34.77\ \cancel{g\ Mn} \times \frac{1\ mol\ Mn}{54.94\ \cancel{g\ Mn}} = 0.6329\ mol\ Mn$$

$$n_O = 40.51\ \cancel{g\ O} \times \frac{1\ mol\ O}{16.00\ \cancel{g\ O}} = 2.532\ mol\ O$$

To begin, assume for simplicity that you have <u>100 g</u> of compound!

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.



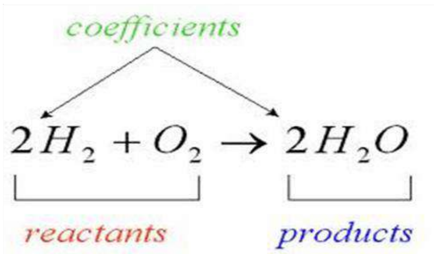
reactants ⟶ products

In a **balanced 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
⟶	Reacts to form products
Δ	The reactants are heated
(*s*)	Solid
(*l*)	Liquid
(*g*)	Gas
(*aq*)	Aqueous

How to "Read" Chemical Equations

$$2\ Mg + O_2 \longrightarrow 2\ MgO$$

2 atoms Mg + 1 molecule O_2 makes 2 formula units MgO

2 moles Mg + 1 mole O_2 makes 2 moles MgO

48.6 grams Mg + 32.0 grams O_2 makes 80.6 g MgO

2 grams Mg + 1 gram O_2 makes 2 g MgO

Balancing Chemical Equations

1. 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

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

2. 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}

Balancing Chemical Equations

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

$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$ — start with C or H but not O

2 carbon on left; 1 carbon on right — multiply CO_2 by 2

$C_2H_6 + O_2 \longrightarrow 2\ CO_2 + H_2O$

6 hydrogen on left; 2 hydrogen on right — multiply H_2O by 3

$C_2H_6 + O_2 \longrightarrow 2\ CO_2 + 3\ H_2O$

Balancing Chemical Equations

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

$C_2H_6 + O_2 \longrightarrow 2\ CO_2 + 3\ H_2O$ — multiply O_2 by $\frac{7}{2}$

2 oxygen on left; 4 oxygen (2x2) + 3 oxygen (3x1) = 7 oxygen on right

$C_2H_6 + \frac{7}{2}O_2 \longrightarrow 2\ CO_2 + 3\ H_2O$ — remove fraction, multiply both sides by 2

$2\ C_2H_6 + 7\ O_2 \longrightarrow 4\ CO_2 + 6\ H_2O$

Balancing Chemical Equations

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

$$2\ C_2H_6 + 7\ O_2 \longrightarrow 4\ CO_2 + 6\ H_2O$$

4 C (2 x 2)	4 C
12 H (2 x 6)	12 H (6 x 2)
14 O (7 x 2)	14 O (4 x 2 + 6)

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

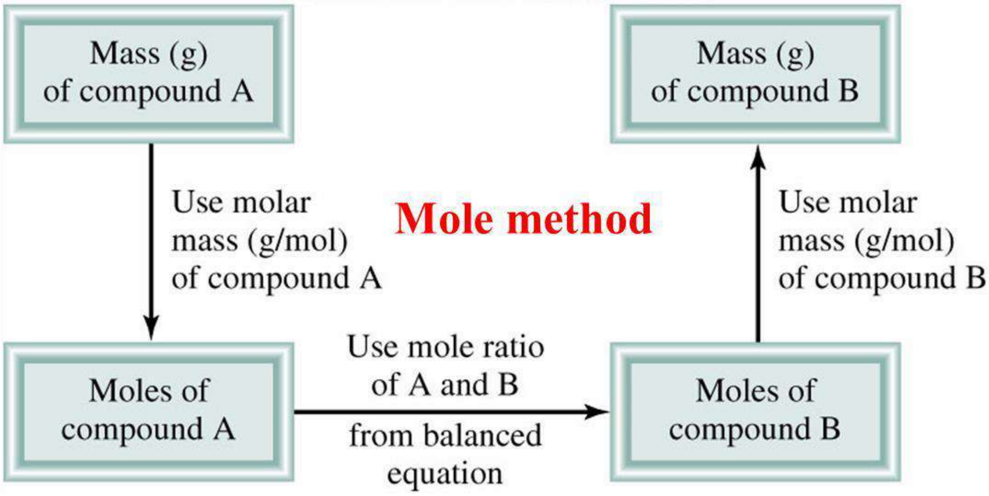
Acetylene gas C_2H_2 burns in the oxyacetylene torch for welding. How many grams of C_2H_2 are burned if the reaction produces 75.0 g CO_2?

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

$$75.0\ g\ CO_2 \times \frac{1\ mole\ CO_2}{44.0\ g\ CO_2} \times \frac{2\ moles\ C_2H_2}{4\ moles\ CO_2} \times \frac{26.0\ g\ C_2H_2}{1\ mole\ C_2H_2}$$

$$= 22.2\ g\ C_2H_2$$

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

$$2\ CH_3OH + 3\ O_2 \longrightarrow 2\ CO_2 + 4\ H_2O$$

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

$$\text{grams } CH_3OH \longrightarrow \text{moles } CH_3OH \longrightarrow \text{moles } H_2O \longrightarrow \text{grams } H_2O$$

$$209\text{ g } CH_3OH \times \frac{1\text{ mol } CH_3OH}{32.0\text{ g } CH_3OH} \times \frac{4\text{ mol } H_2O}{2\text{ mol } CH_3OH} \times \frac{18.0\text{ g } H_2O}{1\text{ mol } H_2O} =$$

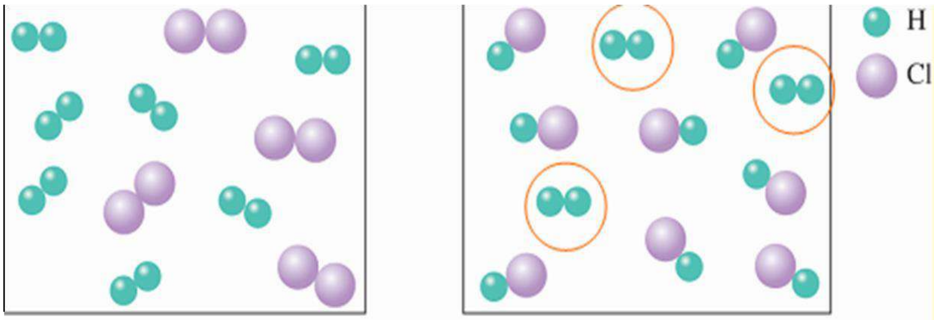
$$235\text{ g of } H_2O$$

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 ⟶ Limiting cars or drivers?
50 chairs + 15 students ⟶ Limiting chairs or students?



(a) Before reaction (b) After reaction

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 ⇒ mol reactant #1 ⇒ mol product ⇒ mass product

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

mass reactant #2 ⇒ mol reactant #2 ⇒ mol product ⇒ mass product

3. The limiting reactant is the reactant that produces the **least** amount of product.

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

$$2\,Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2\,Fe$$

Calculate the mass of Al_2O_3 formed in grams.

1. Balanced reaction: Done.
2. Moles of "given" reactants.

   Moles of Al = 124 g / 26.9815 g/mol = 4.60 mol

   Moles of Fe_2O_3 = 601 g / 159.6882 g/mol = 3.76 mol

3. Moles of "desired" product, Al_2O_3.

$$2\,Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2\,Fe$$

Moles of Al_2O_3 based on Al $= \frac{4.60 \text{ mol Al}}{1} \times \frac{1 \text{ mol } Al_2O_3}{2 \text{ mol Al}} = 2.30 \text{ mol } Al_2O_3$

Moles of Al_2O_3 based on Fe_2O_3 $= \frac{3.76 \text{ mol } Fe_2O_3}{1} \times \frac{1 \text{ mol } Al_2O_3}{1 \text{ mol } Fe_2O_3} = 3.76 \text{ mole } Al_2O_3$

Keep the smaller answer! Al is the limiting reactant.

4. Grams of Al_2O_3 = 2.30 mol X 101.9612 g/mol = **235 g**

How many grams of AgBr can be formed when solutions containing 50 g $MgBr_2$ and 100 g $AgNO_3$ 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 $MgBr_2$ ⟷ 2 mol $AgNO_3$ ⟷ 2 mol AgBr

$$(50/184.1) \text{ mol } MgBr_2 \times \frac{2 \text{ mol AgBr}}{1 \text{ mol } MgBr_2} \times 187.8 = 102 \text{ g AgBr}$$

$$(100/169.9) \text{ mol } AgNO_3 \times \frac{2 \text{ mol AgBr}}{2 \text{ mol } AgNO_3} \times 187.8 = 110.5 \text{ g AgBr}$$

$MgBr_2$ = limiting reactant ⇨ 102 g AgBr is yielded

$$(50/184.1) \text{ mol } MgBr_2 \times \frac{2 \text{ mol } AgNO_3}{1 \text{ mol } MgBr_2} \times 169.9. = 92.3\text{g } AgNO_3$$

100 -92.3 = 7.7 g $AgNO_3$ 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.

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

- Suppose a student performs a reaction and obtains 0.875 g of $CuCO_3$ and the theoretical yield is 0.988 g. What is the percent yield?

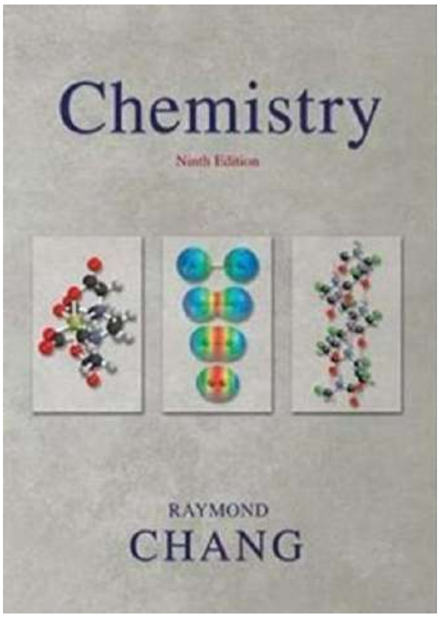
$$Cu(NO_3)_2(aq) + Na_2CO_3(aq) \rightarrow CuCO_3(s) + 2\,NaNO_3(aq)$$

$$\frac{0.875 \text{ g } CuCO_3}{0.988 \text{ g } CuCO_3} \times 100\ \% = 88.6\ \%$$

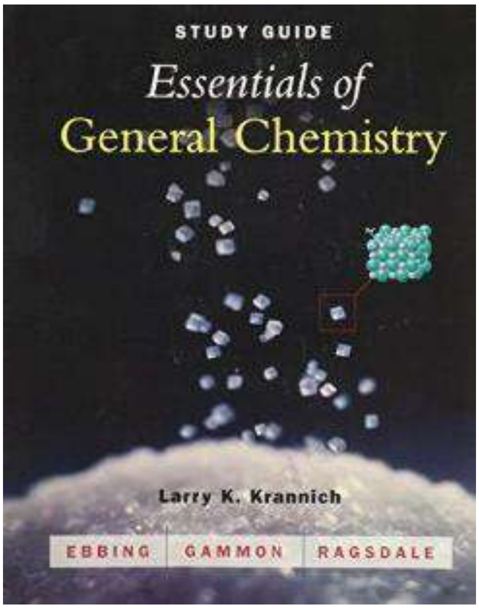
- The percent yield obtained is 88.6%.

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.



2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 4

Reactions in Aqueous Solutions

4.1 General Properties of Aqueous Solutions

4.2 Precipitation Reactions

4.3 Acid- Base Reactions

4.4 Oxidation-Reduction / Redox Reactions

4.5 Concentration of Solutions

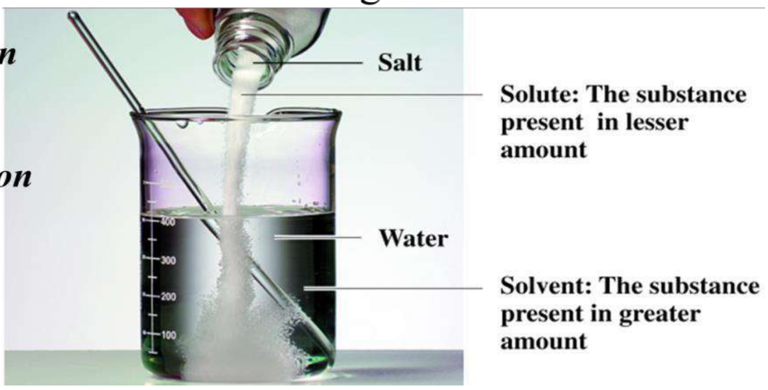
4.6 Titration

4.1 General Properties of Aqueous Solutions

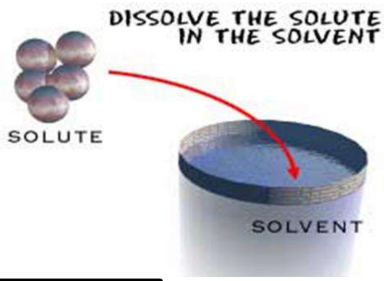
A ***solution*** is a homogenous mixture of 2 or more substances

Solution
- ***solute*** → the substance present in the smaller amount
- \+
- ***solvent*** → the substance present in the larger amount

- → ***Solid Solution***
- → ***Liquid Solution***
- → ***Gas Solution***



Aqueous solution
- solute (gas/liquid/solid)
- \+
- solvent (water)



Solution	Solvent	Solute
Soft drink (*l*)	H_2O	Sugar, CO_2
Air (*g*)	N_2	O_2, CO_2, Ar, CH_4
Alloy (s)	Cu	Ni

Sea water ????

Aqueous Solution	Solvent	Solute
Sea water	H_2O	Salt (NaCl)
Vinegar	H_2O	Acetic acid (CH_3COOH)

Type	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)
	Tincture of iodine	Iodine (solid)	Alcohol
(liquid)			
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

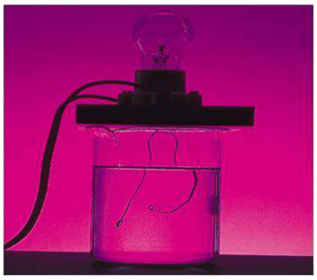
Two types of Solutes

Non-electrolyte

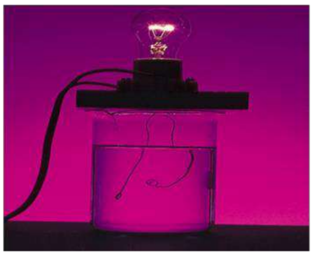
When dissolved in water does not conduct electricity

Electrolyte

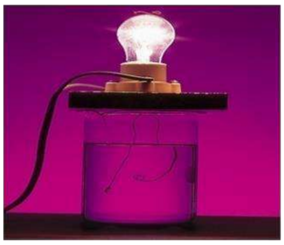
When dissolved in water can conduct electricity



Non-electrolyte



weak electrolyte



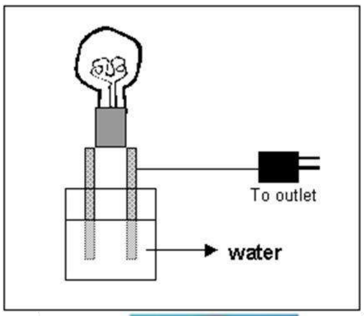
strong electrolyte

Electrolyte conduct electricity in solution?

Dissociation= The splitting of a molecule into smaller molecules, atoms, or ions

Ionization= Separation of atom/molecules into ions

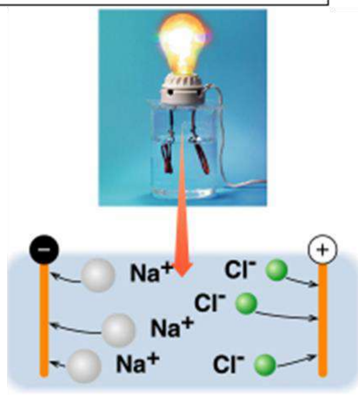
Strong Electrolyte –Complete (100%) dissociation



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

Non-reversible reaction

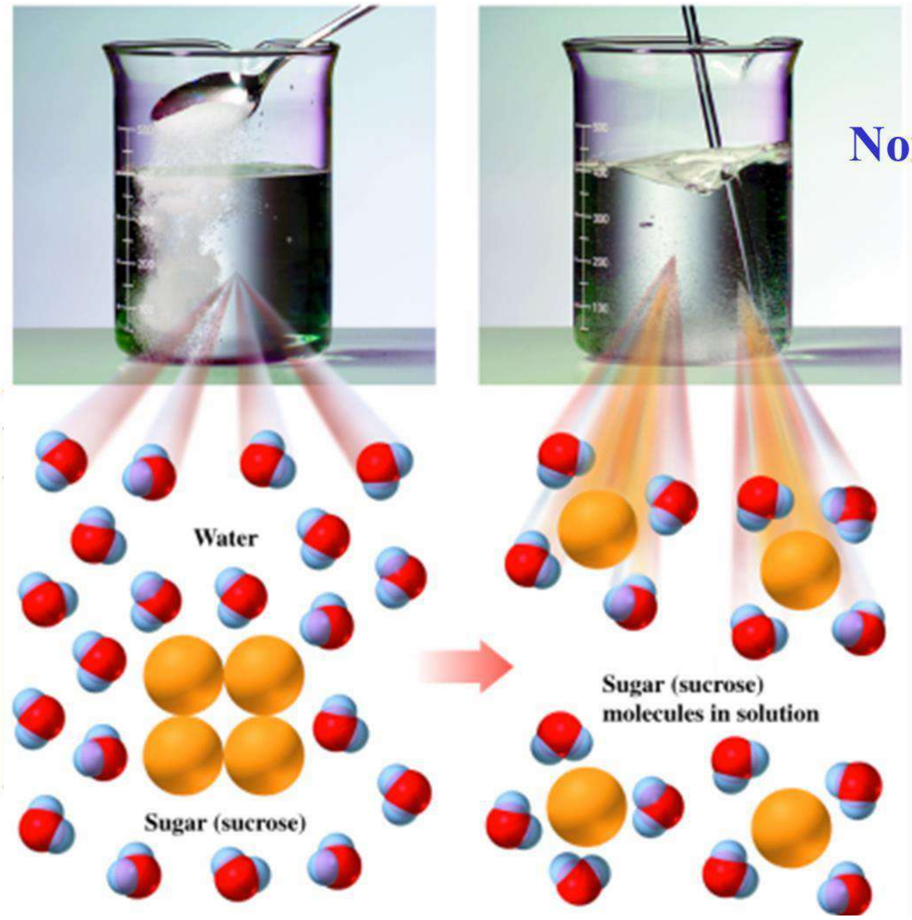
Weak Electrolyte – Incomplete (<100%) dissociation



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

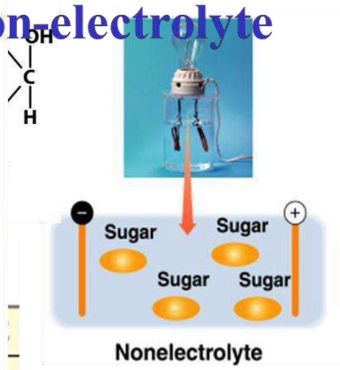
$$CH_3COOH \rightleftharpoons CH_3COO^-\ (aq) + H^+\ (aq)$$

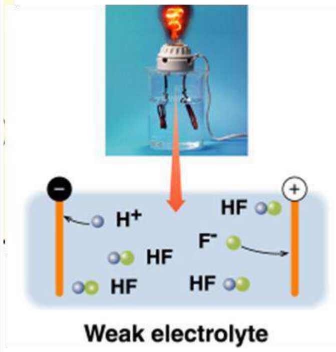
Reversible reaction



?

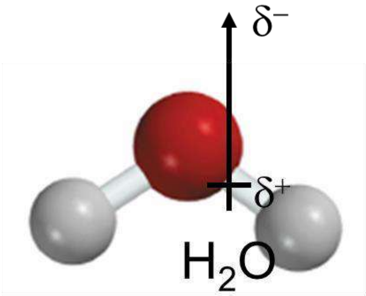
Non-electrolyte





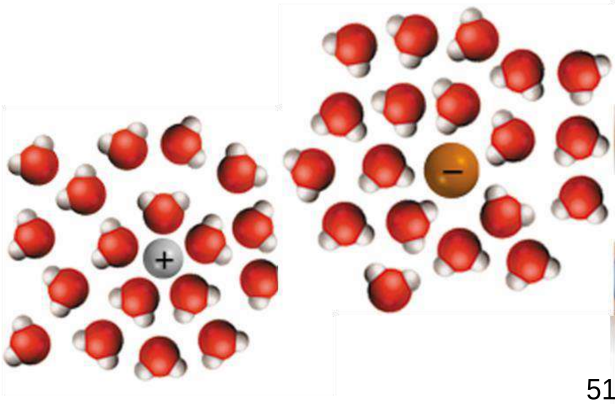
Water

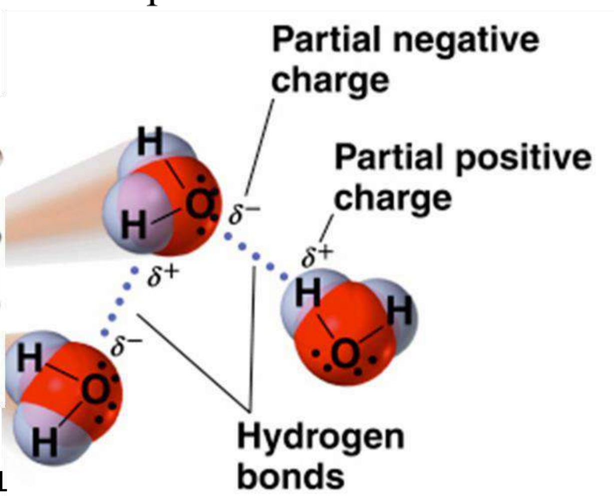
- electrically neutral molecule
- positive and negative region (pole)
- polar solvent (for ionic compounds)



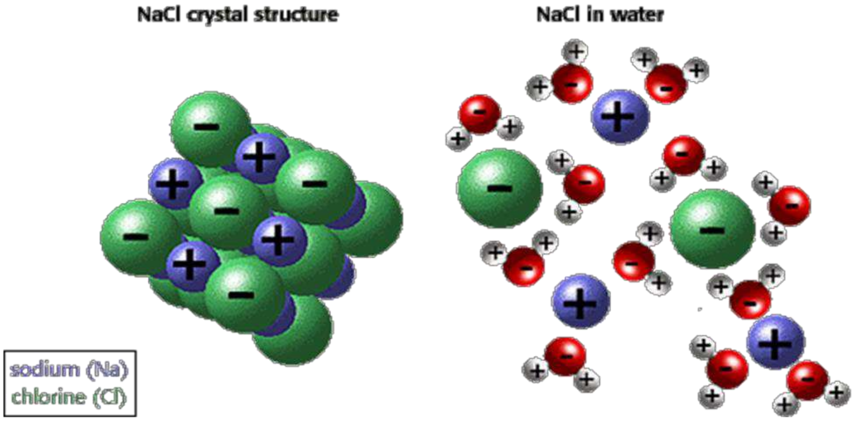
Hydration

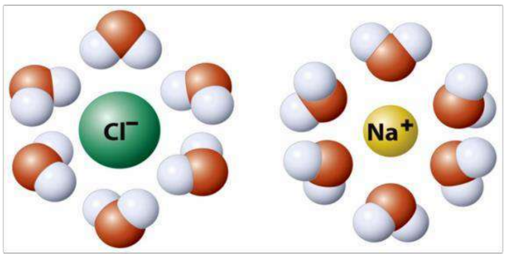
- the process in which an ion is surrounded by water molecules arranged in a specific manner.
- helps to stabilize ions in solution and prevents cations from combining with anions.

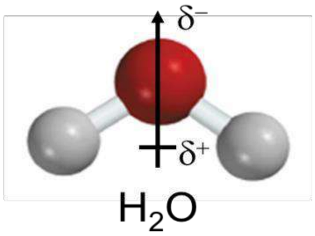




When NaCl dissolves in water, Na^{+} ions and Cl^{-} ions are separated from each other and undergo "hydration".





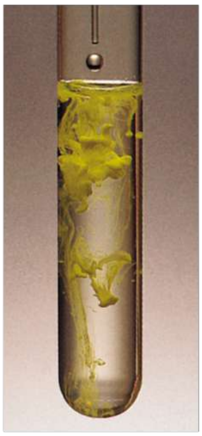


4.2 Precipitation Reactions

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



PbI_2

Example: Precipitation of Lead Iodide

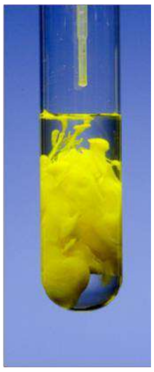
$$Pb(NO_3)_2\ (aq) + 2NaI\ (aq) \longrightarrow PbI_2\ (s) + 2NaNO_3\ (aq)$$

↑ Yellow precipitate (insoluble)

Molecular equation

(species as molecule)

$$Pb(NO_3)_2\,(aq) + 2NaI\,(aq) \longrightarrow PbI_2\,(s) + 2NaNO_3\,(aq)$$



Ionic equation

(species as dissolved free ions)

$$Pb^{2+}\,(aq) + \cancel{2NO_3^-}\,(aq) + \cancel{2Na^+}\,(aq) + 2I^-\,(aq)$$
$$\longrightarrow PbI_2\,(s) + \cancel{2Na^+}\,(aq) + \cancel{2NO_3^-}\,(aq)$$

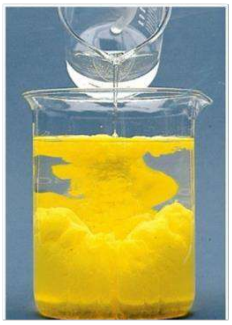
Na^+ and NO_3^- are ***spectator*** ions
(does not involved in the overall reaction)

Net ionic equation

(species that actually take part in the reaction)

$$Pb^{2+}\,(aq) + 2I^-\,(aq) \longrightarrow PbI_2\,(s)$$

PbI_2



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.

$$AgNO_3\,(aq) + NaCl\,(aq) \longrightarrow AgCl\,(s) + NaNO_3\,(aq)$$

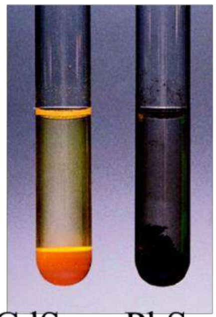
$$Ag^+\,(aq) + \cancel{NO_3^-}\,(aq) + \cancel{Na^+}\,(aq) + Cl^-\,(aq)$$
$$\longrightarrow AgCl\,(s) + \cancel{Na^+}\,(aq) + \cancel{NO_3^-}\,(aq)$$

$$Ag^+\,(aq) + Cl^-\,(aq) \longrightarrow AgCl\,(s)$$

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

Substances ➡ Soluble/ slightly soluble/ insoluble

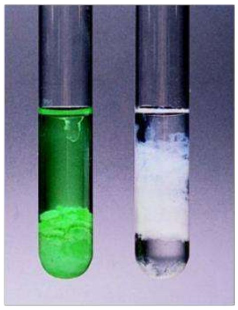
Solubility rules – to predict the solubility of ionic compounds



CdS PbS

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



$Ni(OH)_2$ $Al(OH)_3$

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 H_2.

$$2HCl\ (aq) + Mg\ (s) \longrightarrow MgCl_2\ (aq) + H_2\ (g)$$

- React with carbonates/bicarbonates to produce CO_2

$$2HCl\ (aq) + Na_2CO_3(aq) \longrightarrow 2NaCl\ (aq) + CO_2\ (g) + H_2O\ (l)$$

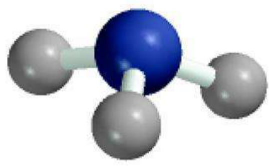
- Aqueous acid solutions conduct electricity.

Properties of Bases

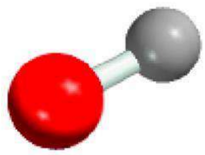
- Substance that ionize in water to produce OH- ion (Arrhenius)

- Have a bitter taste.
- Feel slippery. Many soaps contain bases.
- Change litmus from red to blue

- Aqueous base solutions conduct electricity.

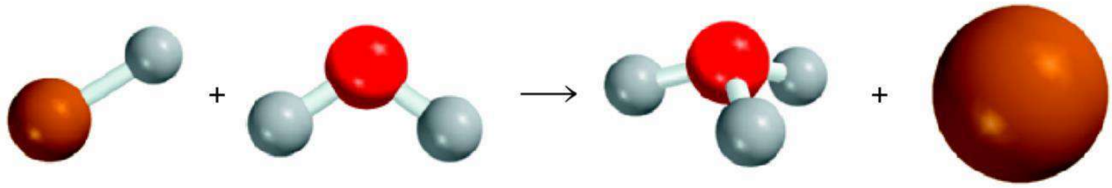


NH_3



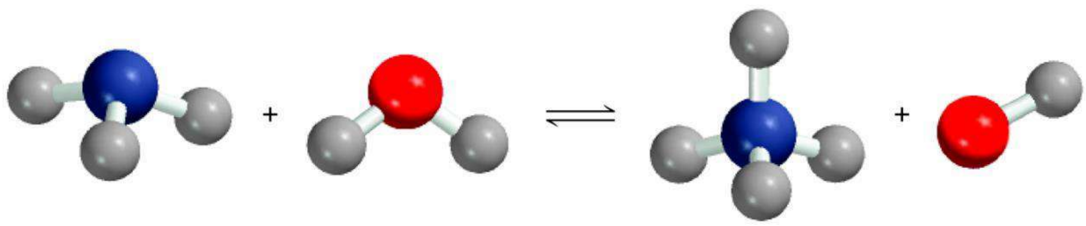
OH^-

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



$HCl + H_2O \longrightarrow H_3O^+ + Cl^-$

Arrhenius base is a substance that produces OH^- in water



$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^-$

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

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

HCl is Bronsted acid because it donates proton

$$HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$$

$$HCl(aq) + H_2O(l) \longrightarrow H_3O^+(aq) + Cl^-(aq)$$

H_3O^+ = Hydrated proton (Hydronium)

NH_3 is Bronsted base because it accepts proton

$$NH_3\ (aq) + H^+\ (aq) \rightleftharpoons NH_4^+\ (aq)$$

$$NH_3\ (aq) + H_2O\ (l) \rightleftharpoons NH_4^+\ (aq) + OH^-\ (aq)$$

TABLE 4.3

Some Common Strong and Weak Acids

Strong Acids		Weak Acids	
Hydrochloric acid	HCl	Hydrofluoric acid	HF
Hydrobromic acid	HBr	Nitrous acid	HNO_2
Hydroiodic acid	HI	Phosphoric acid	H_3PO_4
Nitric acid	HNO_3	Acetic acid	CH_3COOH
Sulfuric acid	H_2SO_4		
Perchloric acid	$HClO_4$		

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

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

$H_2PO_4^-\ (aq) \rightleftharpoons H^+\ (aq) + HPO_4^{2-}\ (aq)$ 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 .

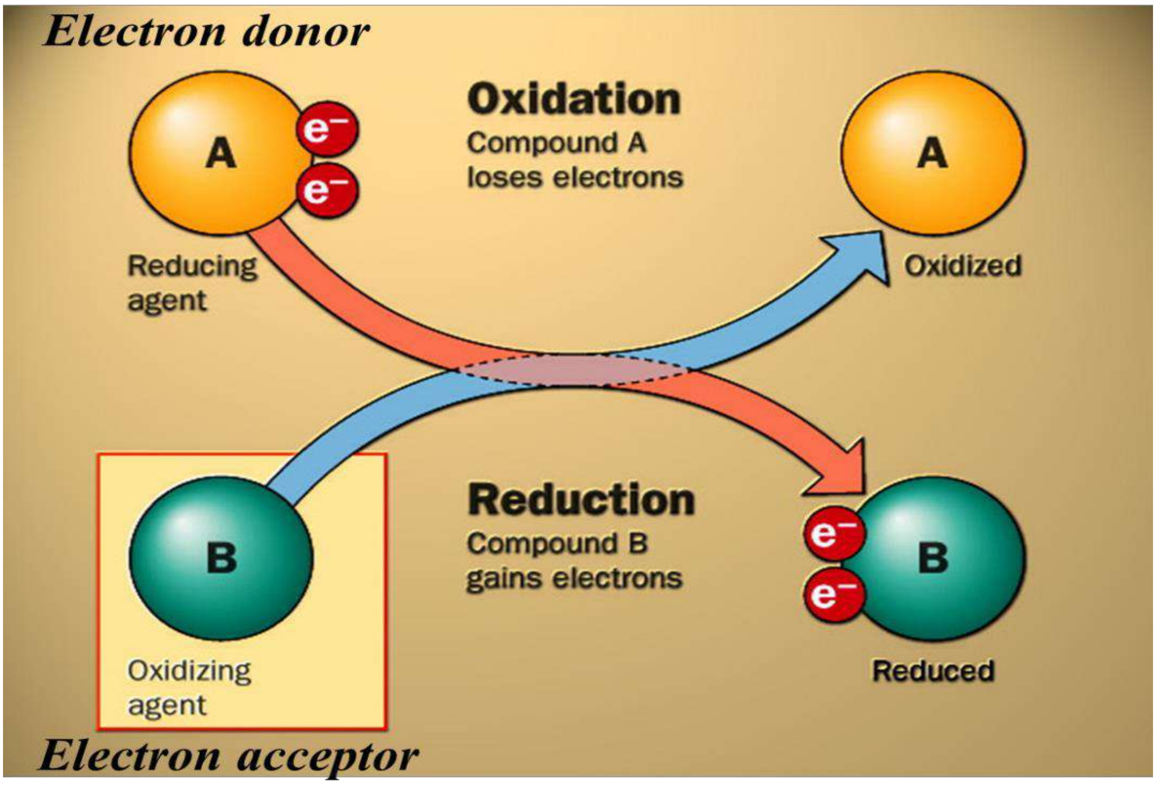
acid + base ⟶ salt + water

$HCl\ (aq) + NaOH\ (aq) \longrightarrow NaCl\ (aq) + H_2O(l)$

$H^+\ (aq) + \cancel{Cl^-}\ (aq) + \cancel{Na^+}\ (aq) + OH^-\ (aq) \longrightarrow \cancel{Na^+\ (aq)} + \cancel{Cl^-\ (aq)} + H_2O\ (l)$

$H^+\ (aq) + OH^-\ (aq) \longrightarrow H_2O\ (l)$

4.4 Oxidation-Reduction / Redox Reactions



Oxidation-Reduction / Redox Reactions

(electron transfer reactions)

Example: formation of MgO from Mg and O_2

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

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

$$2Mg + O_2 + \cancel{4e^-} \longrightarrow 2Mg^{2+} + 2O^{2-} + \cancel{4e^-}$$

$$2Mg + O_2 \longrightarrow 2MgO$$

Oxidized (2Mg)

Reduced (O_2)

Reducing Agent: donates electrons to O_2 and causes O_2 to be reduced

Oxidizing Agent: accepts electrons from Mg and causes Mg to be oxidized

$$Zn\ (s) + CuSO_4\ (aq) \longrightarrow ZnSO_4\ (aq) + Cu\ (s)$$

$Zn \longrightarrow Zn^{2+} + 2e^-$ Zn is oxidized Zn is the ***reducing agent***

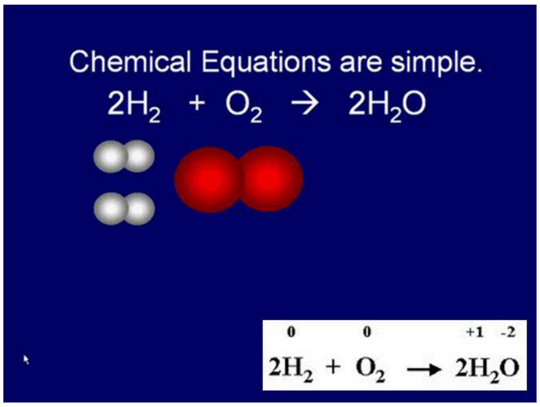
$Cu^{2+} + 2e^- \longrightarrow Cu$ Cu^{2+} is reduced Cu^{2+} is the ***oxidizing agent***

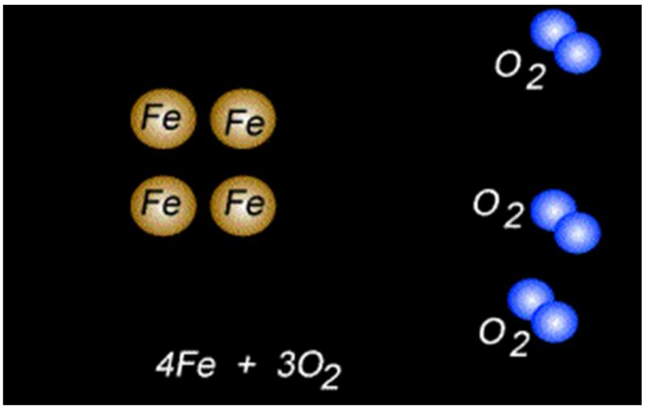
Copper wire reacts with silver nitrate to form silver metal.
What is the oxidizing agent in the reaction?

$$Cu\ (s) + 2AgNO_3\ (aq) \longrightarrow Cu(NO_3)_2\ (aq) + 2Ag\ (s)$$

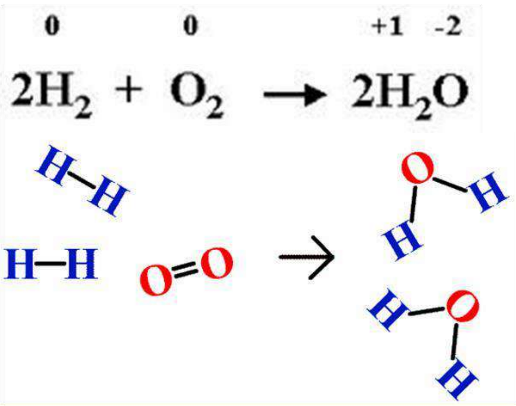
$Cu \longrightarrow Cu^{2+} + 2e^-$ Cu is oxidized Cu is the ***reducing agent***

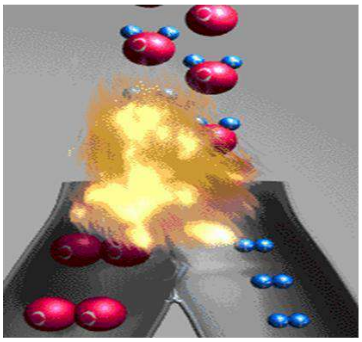
$Ag^+ + 1e^- \longrightarrow Ag$ Ag^+ is reduced Ag^+ is the **oxidizing agent**

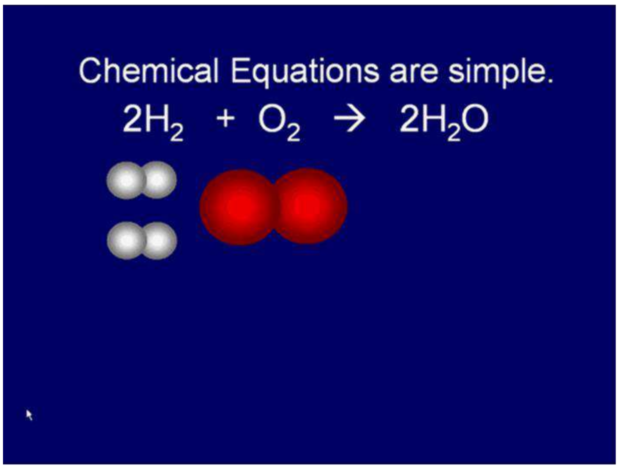


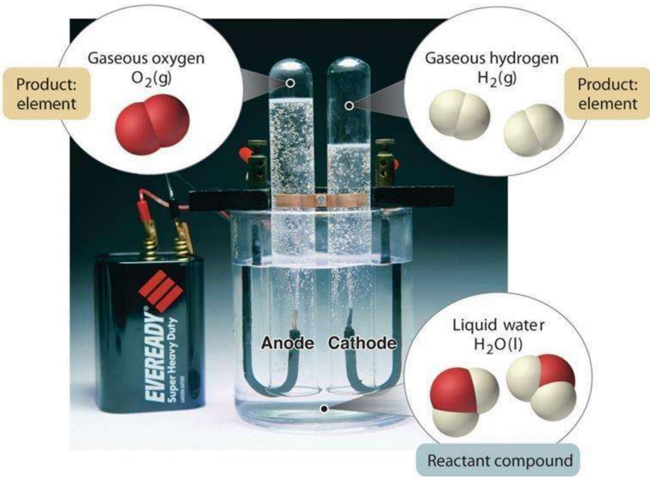


Hydrogen and oxygen react chemically to form water

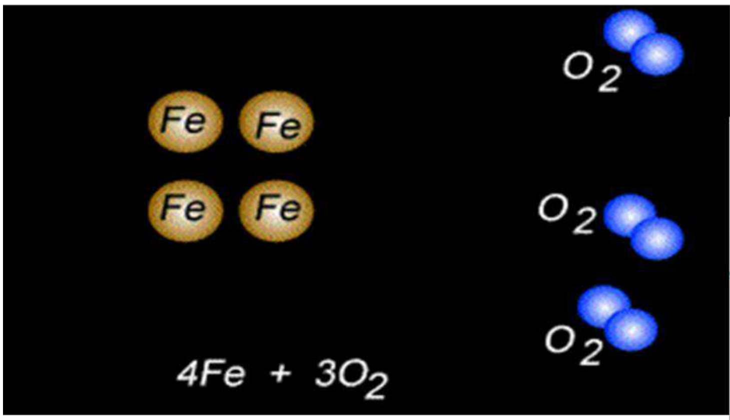


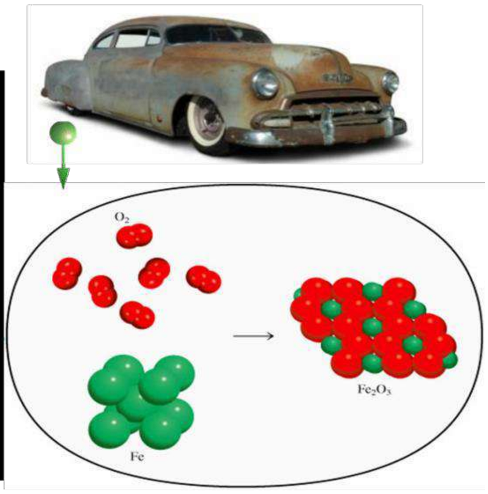






Rusting





Oxidation number

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

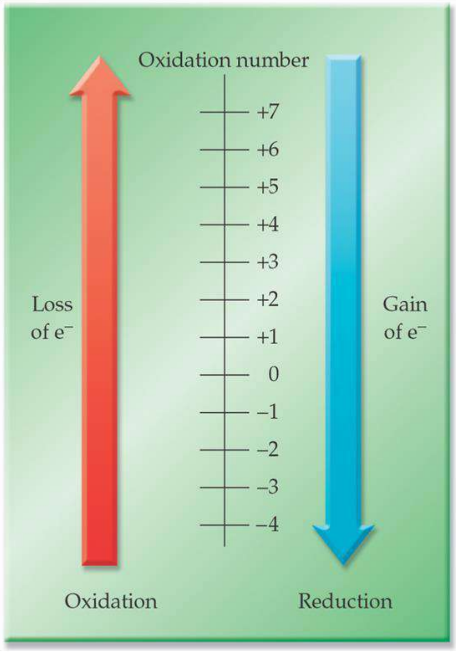
1. Free elements (uncombined state) have an oxidation number of zero.

   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.

   Li^+ = +1; Fe^{3+} = +3; O^{2-} = -2

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, CaH_2). In these cases, its oxidation number is –1

5. 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 –½.

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

HCO_3^- IF_7 $NaIO_3$ $K_2Cr_2O_7$

The Oxidation Numbers of Elements in their Compounds

- Metallic element: +ve oxidation numbers
- Non-metallic elements: +ve/-ve oxidation numbers
- Elements in group 1A-7A can have oxidation numbers=group number
- Transition metals have many possible oxidation numbers

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 **H** +1 −1																	2 **He**
3 **Li** +1	4 **Be** +2											5 **B** +3	6 **C** +4 +2 −4	7 **N** +5 +4 +3 +2 +1 −3	8 **O** +2 $-\frac{1}{2}$ −1 −2	9 **F** −1	10 **Ne**
11 **Na** +1	12 **Mg** +2											13 **Al** +3	14 **Si** +4 −4	15 **P** +5 +3 −3	16 **S** +6 +4 +2 −2	17 **Cl** +7 +6 +5 +4 +3 +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 +4	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

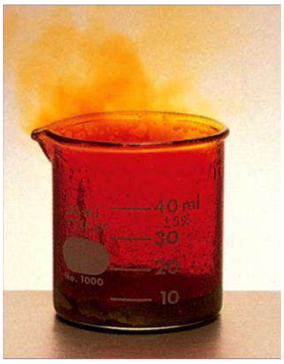
Oxidation	Aspect	Reduction
Loss of electrons	Gain/loss of electron	**Gain electrons**
Increase in oxidation number	Increase/decrease in oxidation number	**Decrease in oxidation number**

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.

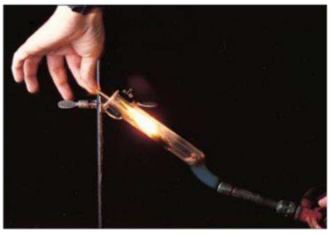


$$A + B \longrightarrow C$$

$$\overset{0}{2Al} + \overset{0}{3Br_2} \longrightarrow \overset{+3\ -1}{2AlBr_3}$$

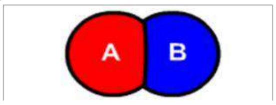
Decomposition Reaction

Breakdown of a compound into two or more components.



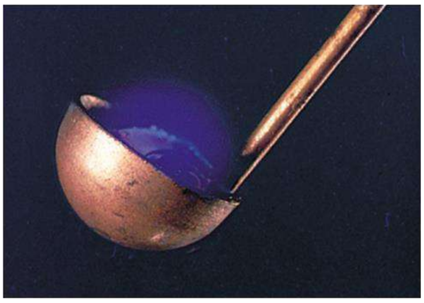
$$C \longrightarrow A + B$$

$$\overset{+1\ +5\ -2}{2KClO_3} \longrightarrow \overset{+1\ -1}{2KCl} + \overset{0}{3O_2}$$



Combustion Reaction

Reaction of a substance with oxygen, usually with the release of heat and light to produce a flame



$$A + O_2 \longrightarrow B$$

$$\overset{0}{S} + \overset{0}{O_2} \longrightarrow \overset{+4\ -2}{SO_2}$$

$$\overset{0}{2Mg} + \overset{0}{O_2} \longrightarrow \overset{+2\ -2}{2MgO}$$

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

$$\overset{0}{Ca} + 2\overset{+1}{H_2}O \longrightarrow \overset{+2}{Ca}(OH)_2 + \overset{0}{H_2}$$

$$\overset{0}{Zn} + 2\overset{+1}{H}Cl \longrightarrow \overset{+2}{Zn}Cl_2 + \overset{0}{H_2}$$

2. Metal Displacement

Displace of metal by another metal

$$\overset{+4}{Ti}Cl_4 + 2\overset{0}{Mg} \longrightarrow \overset{0}{Ti} + 2\overset{+2}{Mg}Cl_2$$

$$\overset{0}{Zn} + \overset{+2}{Cu}SO_4 \longrightarrow \overset{+2}{Zn}SO_4 + \overset{0}{Cu}$$

The Activity Series for Metals

(the strength as reducing agent)

$$2K + 2H_2O \longrightarrow 2KOH + H_2 \text{ (fast)}$$

$$Mg + 2H_2O \longrightarrow Mg(OH)_2 + H_2 \text{(slow)}$$

$$Cu + 2H_2O \longrightarrow \text{no reaction}$$

Reactivity
K > Mg > Cu

Reducing strength increases (from bottom to top)

$Li \rightarrow Li^{+} + e^{-}$	React with cold water to produce H_2
$K \rightarrow K^{+} + e^{-}$	
$Ba \rightarrow Ba^{2+} + 2e^{-}$	
$Ca \rightarrow Ca^{2+} + 2e^{-}$	
$Na \rightarrow Na^{+} + e^{-}$	
$Mg \rightarrow Mg^{2+} + 2e^{-}$	React with steam to produce H_2
$Al \rightarrow Al^{3+} + 3e^{-}$	
$Zn \rightarrow Zn^{2+} + 2e^{-}$	
$Cr \rightarrow Cr^{3+} + 3e^{-}$	
$Fe \rightarrow Fe^{2+} + 2e^{-}$	
$Cd \rightarrow Cd^{2+} + 2e^{-}$	
$Co \rightarrow Co^{2+} + 2e^{-}$	React with acids to produce H_2
$Ni \rightarrow Ni^{2+} + 2e^{-}$	
$Sn \rightarrow Sn^{2+} + 2e^{-}$	
$Pb \rightarrow Pb^{2+} + 2e^{-}$	
$H_2 \rightarrow 2H^{+} + 2e^{-}$	
$Cu \rightarrow Cu^{2+} + 2e^{-}$	Do not react with water or acids to produce H_2
$Ag \rightarrow Ag^{+} + e^{-}$	
$Hg \rightarrow Hg^{2+} + 2e^{-}$	
$Pt \rightarrow Pt^{2+} + 2e^{-}$	
$Au \rightarrow Au^{3+} + 3e^{-}$	

3. Halogen Displacement Reaction

Displace of halogen by another halogen

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

$F_2 > Cl_2 > Br_2 > I_2$

$$\overset{0}{Cl_2} + 2K\overset{-1}{Br} \longrightarrow 2K\overset{-1}{Cl} + \overset{0}{Br_2}$$

$$\overset{0}{Cl_2} + 2Na\overset{-1}{I} \longrightarrow 2Na\overset{-1}{Cl} + \overset{0}{I_2}$$

$$I_2 + KBr \longrightarrow \text{no reaction}$$

4. Disproportionation Reaction

The same element is simultaneously oxidized and reduced.

reduced

$$\overset{0}{Cl_2} + 2OH^- \longrightarrow \overset{+1}{Cl}O^- + \overset{-1}{Cl^-} + H_2O$$

oxidized

Classify each of the following reactions.

$$Ca^{2+} + CO_3^{2-} \longrightarrow CaCO_3$$ Precipitation

$$BaCl_2 + NaSO_4 \longrightarrow NaCl_2 + BaSO_4$$ Metathesis/ Double displacement

$$Zn + 2HCl \longrightarrow ZnCl_2 + H_2$$ Redox (H_2 Displacement)

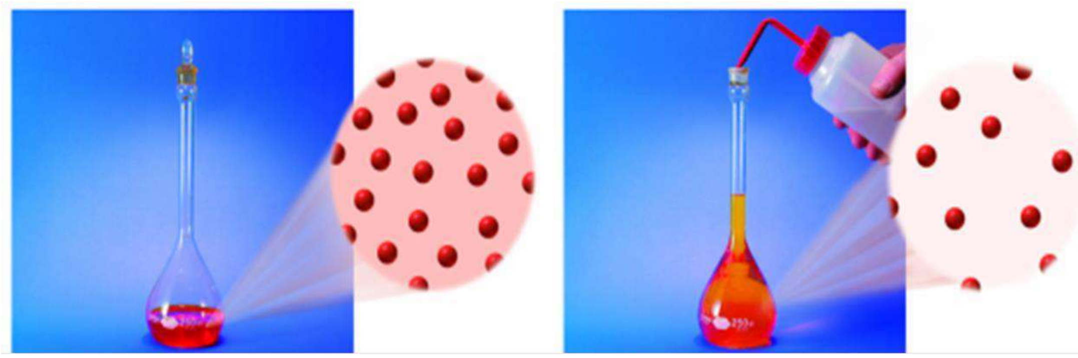
$$Ca + F_2 \longrightarrow CaF_2$$ Redox (Combination)

$$2H_2O \longrightarrow O_2 + 2H_2$$ Redox (decomposition)

$$2H_2O_2 \longrightarrow 2H_2O + O_2$$ Redox (disproportionation)

-1 -2 0

4.5 Concentration of Solutions



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

Molarity/ molar concentration (M)

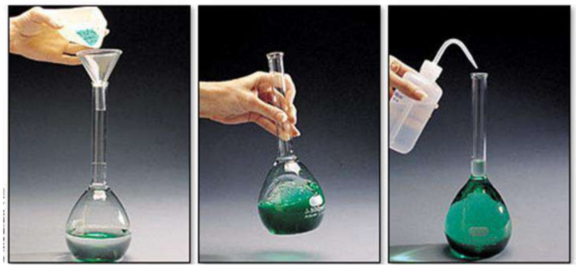
The number of moles of solute in 1 liter (L) of solution

Unit= moles/liter (mol/L)

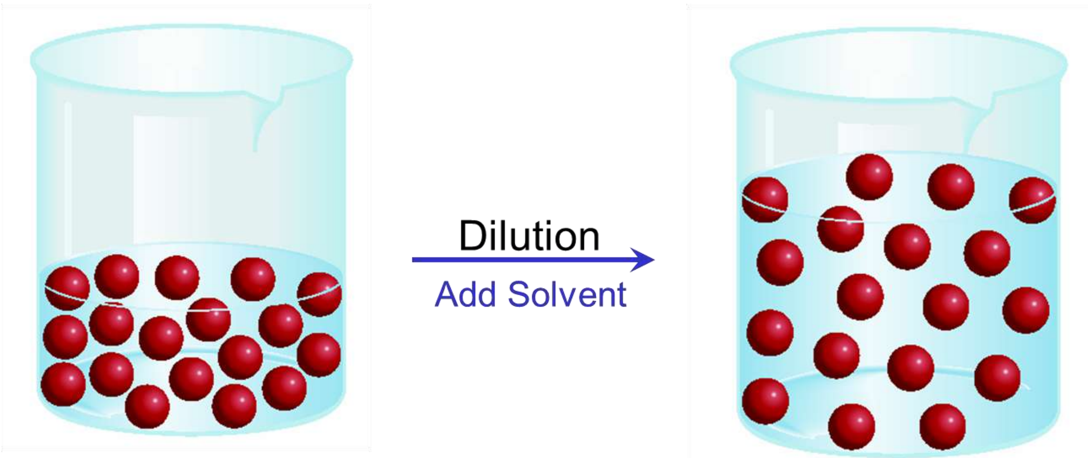
$$M = molarity = \frac{\text{moles of solute (mol)}}{\text{liters of solution (L)}}$$

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

$$\text{moles} = \text{molarity (mol/L)} \times \text{volume (L)}$$
$$= MV$$



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



Moles of solute before dilution (i) = Moles of solute after dilution (f)

$$M_iV_i = M_fV_f$$

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

$$\text{volume of KI solution} \xrightarrow{M\ \text{KI}} \text{moles KI} \xrightarrow{\mathcal{M}\ \text{KI}} \text{grams KI}$$

$$500.\ \text{mL} \times \frac{1\ \text{L}}{1000\ \text{mL}} \times \frac{2.80\ \text{mol KI}}{1\ \text{L soln}} \times \frac{166\ \text{g KI}}{1\ \text{mol KI}} = 232\ \text{g KI}$$

How would you prepare 60.0 mL of 0.200 *M* HNO_3 from a stock solution of 4.00 *M* HNO_3?

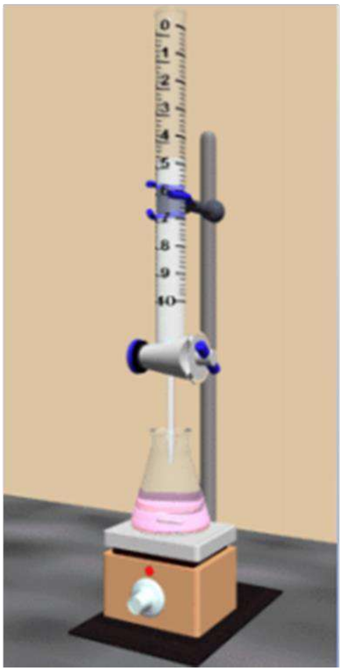
$$M_i V_i = M_f V_f$$

$M_i = 4.00\ M$ $M_f = 0.200\ M$ $V_f = 0.0600\ \text{L}$ $V_i = ?\ \text{L}$

$$V_i = \frac{M_f V_f}{M_i} = \frac{0.200\ M \times 0.0600\ \text{L}}{4.00\ M} = 0.00300\ \text{L} = 3.00\ \text{mL}$$

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

4.6 Titration



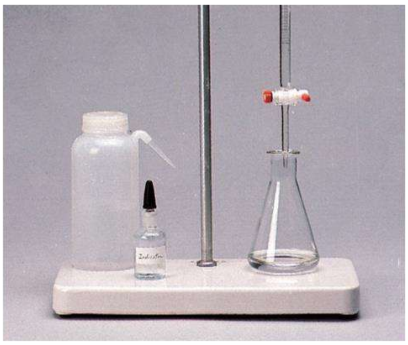
Titrations -A solution of **known concentration** (standard solution) is added gradually to another solution of **unknown concentration** until the **chemical reaction** between the two solutions is **complete**.

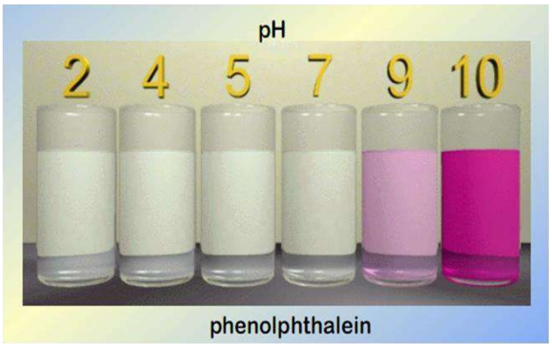
Equivalence point – the point at which the reaction is complete

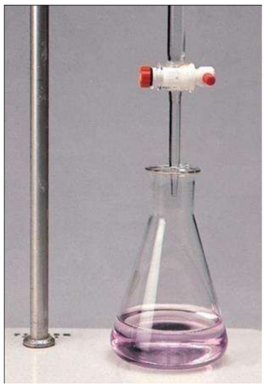
End point – the point at which the indicator permanently changes its color

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^-)

$$\mathbf{10\ FeSO_4 + 2\ KMnO_4 + 8\ H_2SO_4 \longrightarrow 5\ Fe_2(SO_4)_3 + 2\ MnSO_4 + K_2SO_4 + 8\ H_2O}$$

$$5Fe^{2+} + MnO_4^- + 8H^+ \longrightarrow 5Fe^{3+} + Mn^{2+} + 4H_2O$$

What volume of a 1.420 *M* NaOH solution is required to titrate 25.00 mL of a 4.50 *M* H_2SO_4 solution?

$$H_2SO_4 + 2NaOH \longrightarrow 2H_2O + Na_2SO_4$$

$$\text{volume acid} \xrightarrow[\text{acid}]{M} \text{moles acid} \xrightarrow[\text{coef.}]{\text{rxn}} \text{moles base} \xrightarrow[\text{base}]{M} \text{volume base}$$

$$25.00\ \text{mL} \times \frac{4.50\ \text{mol}\ H_2SO_4}{1000\ \text{mL soln}} \times \frac{2\ \text{mol NaOH}}{1\ \text{mol}\ H_2SO_4} \times \frac{1000\ \text{ml soln}}{1.420\ \text{mol NaOH}} = 158\ \text{mL}$$

16.42 mL of 0.1327 *M* $KMnO_4$ solution is needed to oxidize 25.00 mL of an acidic $FeSO_4$ solution. What is the molarity of the iron solution?

$$5Fe^{2+} + MnO_4^- + 8H^+ \longrightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O$$

$$\text{volume red} \xrightarrow[\text{red}]{M} \text{moles red} \xrightarrow[\text{coef.}]{\text{rxn}} \text{moles oxid} \xrightarrow[\text{oxid}]{V} M\ \text{oxid}$$

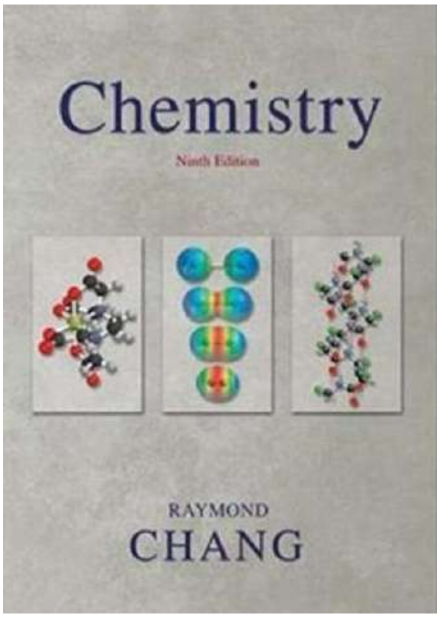
16.42 mL = 0.01642 L

25.00 mL = 0.02500 L

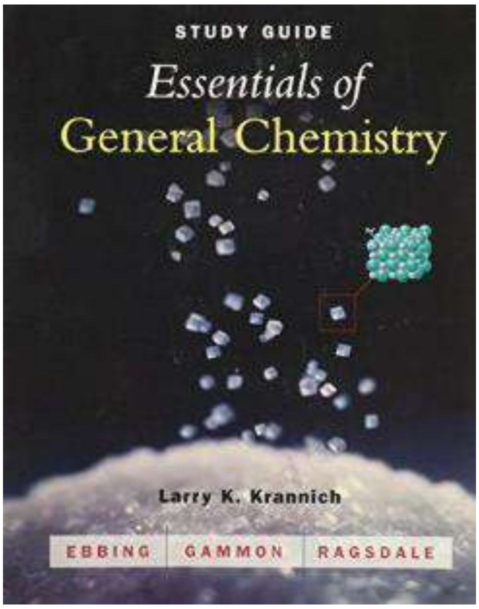
$$0.01642\ \cancel{L} \times \frac{0.1327\ \cancel{mol\ KMnO_4}}{1\ \cancel{L}} \times \frac{5\ mol\ Fe^{2+}}{1\ \cancel{mol\ KMnO_4}} \times \frac{1}{0.02500\ L\ Fe^{2+}} = 0.436\ M$$

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.

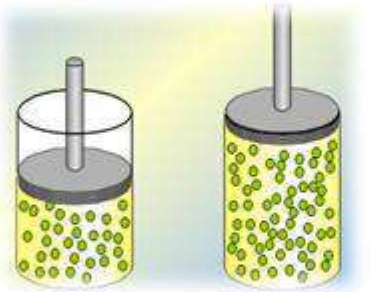


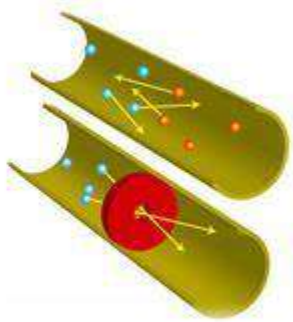
2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 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

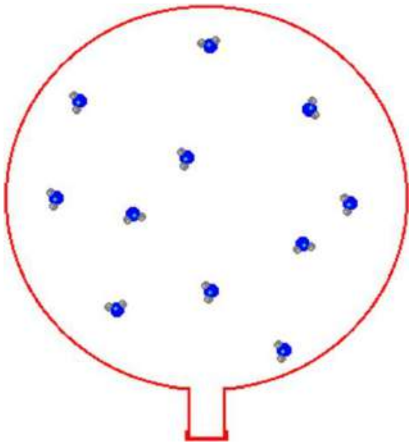
5.5 Gas Stoichiometry

5.6 Dalton's Law of Partial Pressures

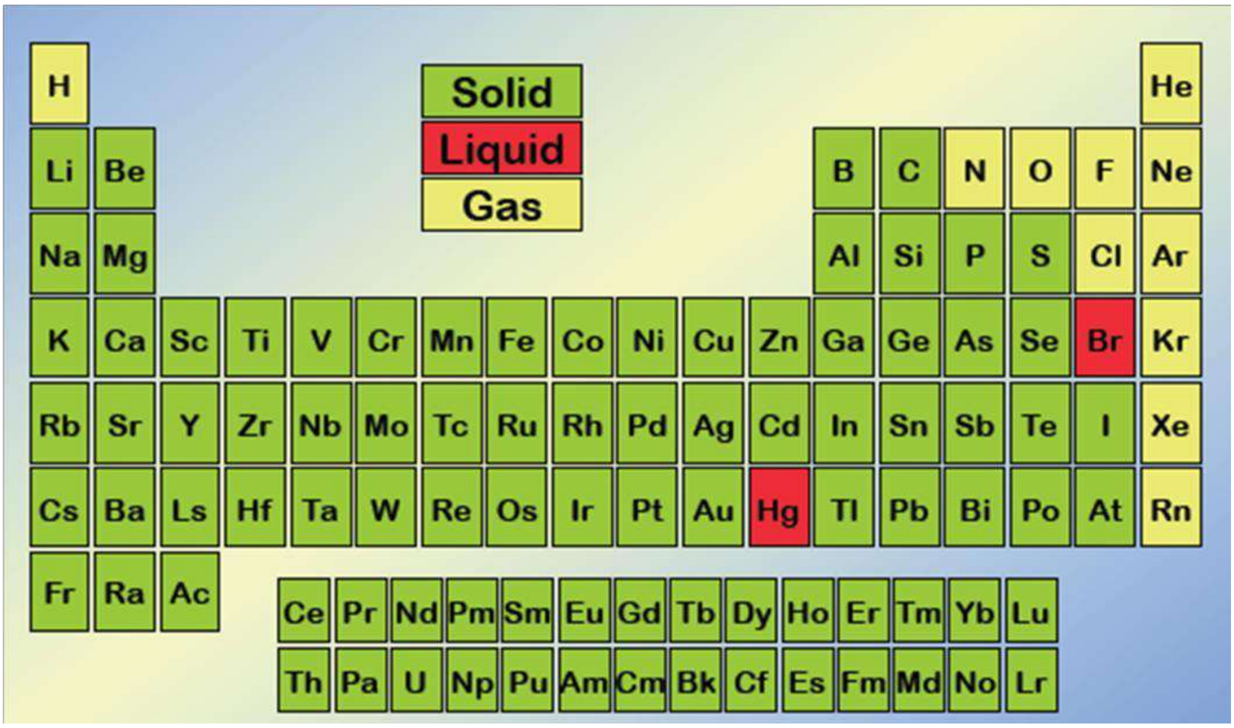
5.7 The Kinetic Molecular Theory of Gases

5.8 Deviation From Ideal Behavior

5.1 Substances That Exist As Gases



Elemental state at 25^0C 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

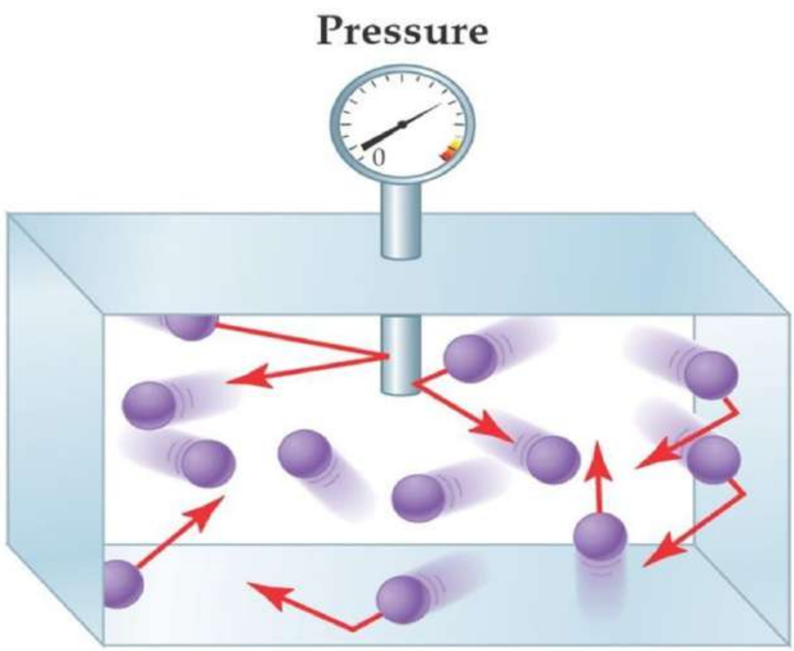
Property	State: Solid	State: Liquid	State: Gas
Density	High	High (like solids)	Low
Shape	Fixed	Takes shape of low part of container	Expands to fill the container
Compressibility	Small	Small	Large

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_2O (nitrous oxide)
Xe (xenon)	SO_2 (sulfur dioxide)
Rn (radon)	H_2S (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.

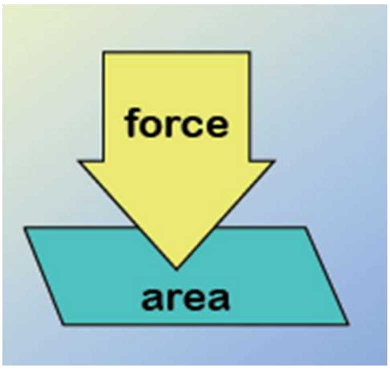
5.2 Pressure of A Gas



Pressure of a gas

$$\text{Pressure} = \frac{\text{Force}}{\text{Area}} = \frac{\text{kg m/s}^2}{\text{m}^2} = \frac{N}{\text{m}^2}$$

(force = mass x acceleration)
= kg m/s^2



SI Units of Pressure

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

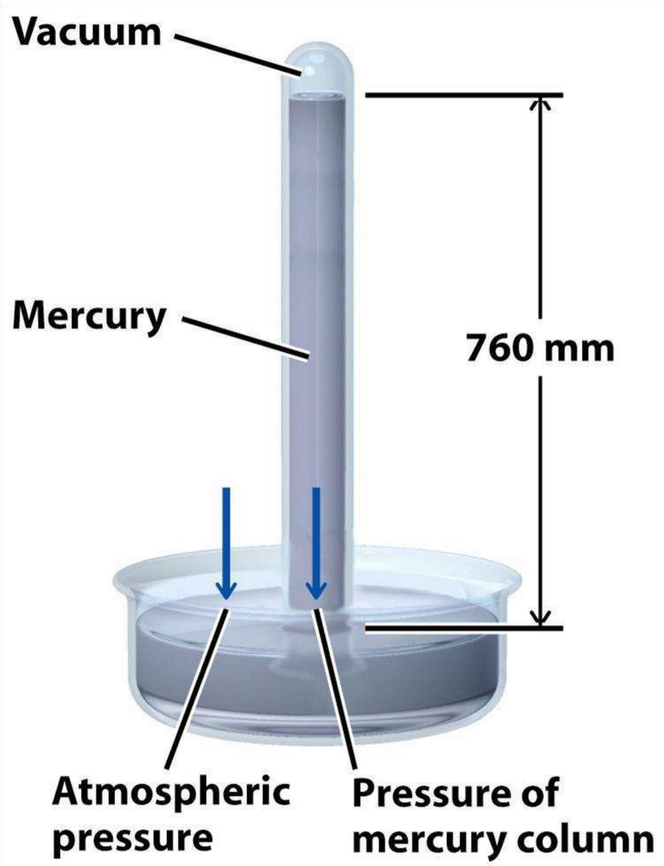
1 pascal (Pa) = 1 N/m^2

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.

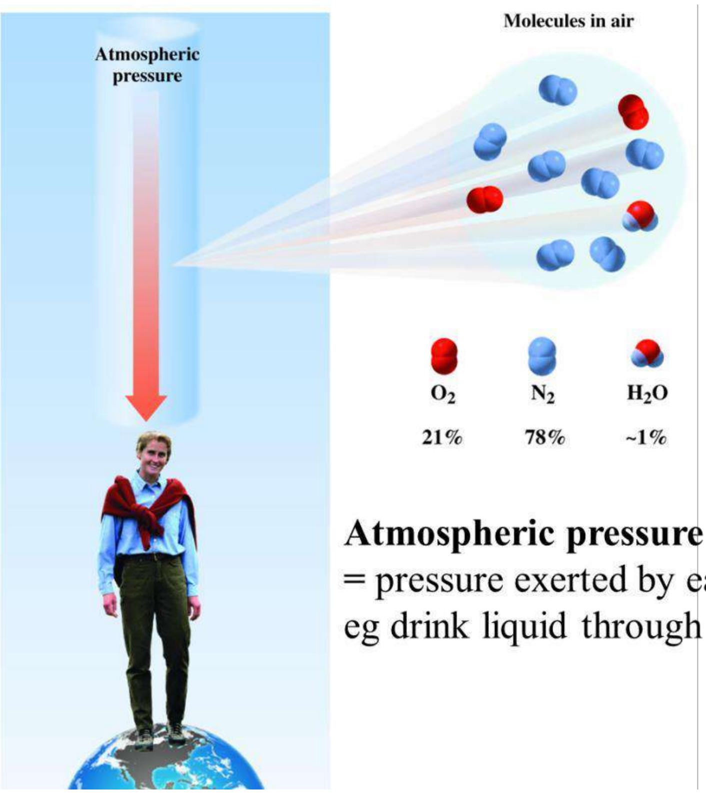


A. What is 475 mm Hg expressed in atm?

$$475 \text{ }\cancel{\text{mm}}\text{ Hg} \times \frac{1 \text{ atm}}{760 \text{ }\cancel{\text{mm}}\text{ Hg}} = 0.625 \text{ atm}$$

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

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



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

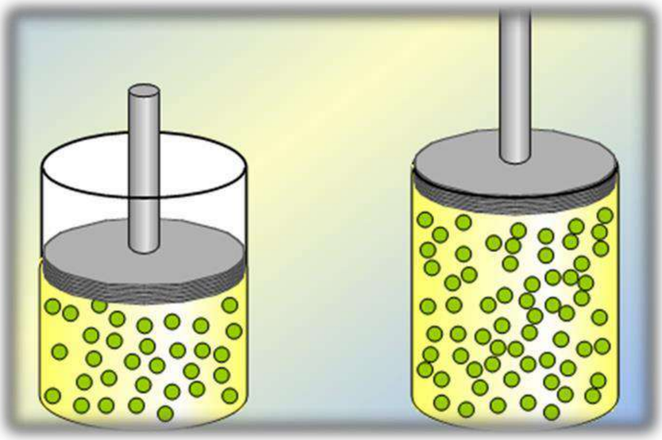
Properties That Describe a Gas

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 ***number of molecules*** 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

$$V \propto \frac{1}{P}$$

T constant
n constant

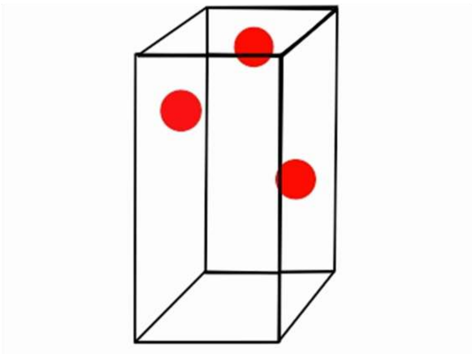
$$V = K\frac{1}{P}$$

K= proportionality constant

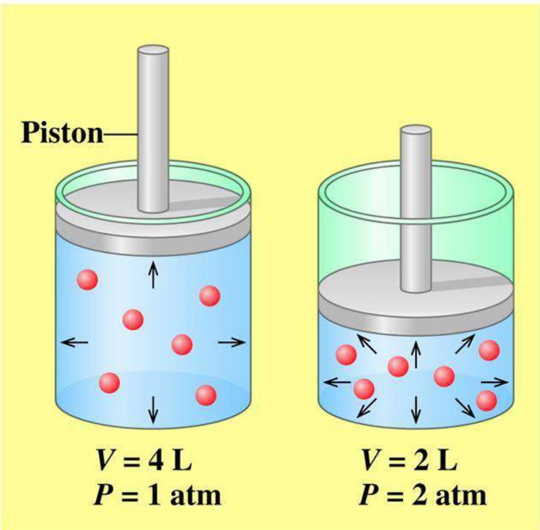
$$P \times V = K$$

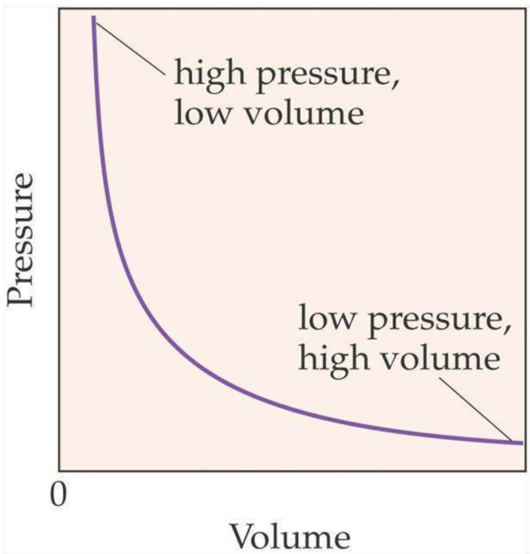
$$P_1V_1 = K = P_2V_2$$

$$P_1V_1 = P_2V_2$$



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?

$$P \text{ x } V = constant$$

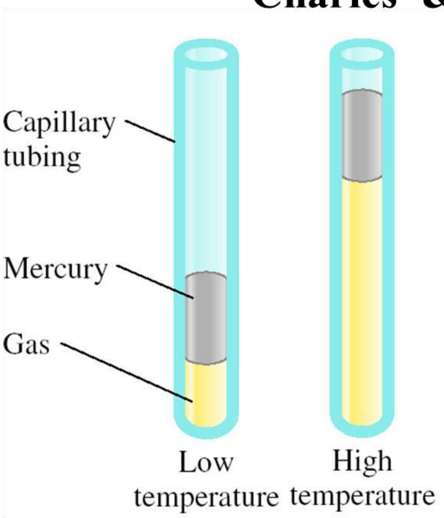
$$P_1 \text{ x } V_1 = P_2 \text{ x } V_2$$

P_1 = 726 mmHg $\qquad$ P_2 = ?

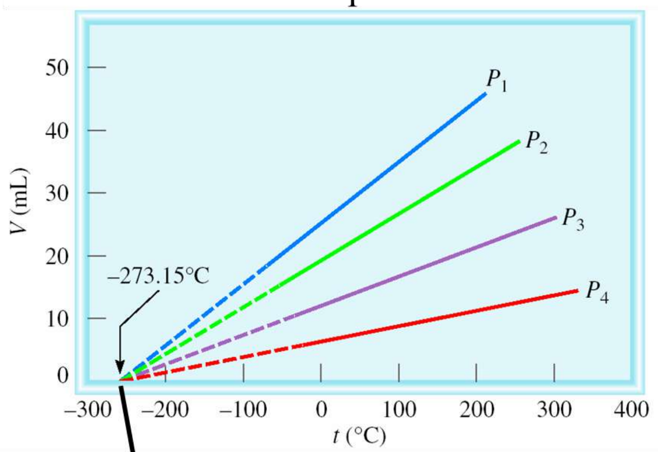
V_1 = 946 mL $\qquad$ V_2 = 154 mL

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

Charles' & Gay-Lussac's Law



temperature-volume relationship at various pressures



As T increases, V increases

-273.15 ^{0}C = Absolute zero

↓

T (K) = t (^{0}C) + 273.15 $\qquad$ Kelvin temperature scale

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

$V \propto T$

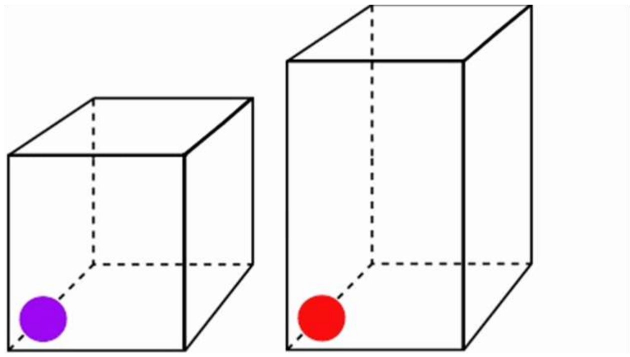
P and n are constant

$V = kT$ or $\frac{V}{T} = k$

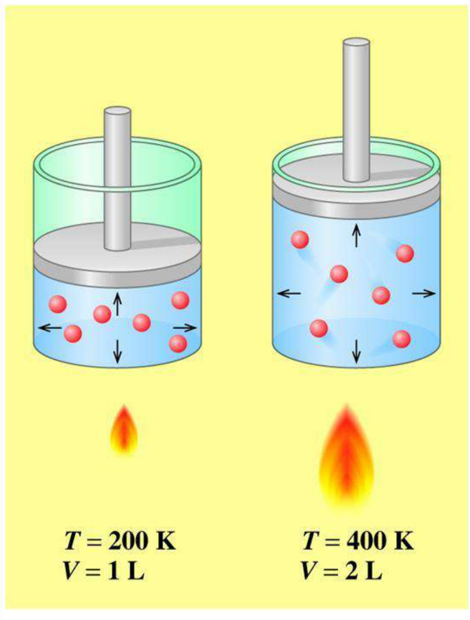
Temperature **must** be in Kelvin

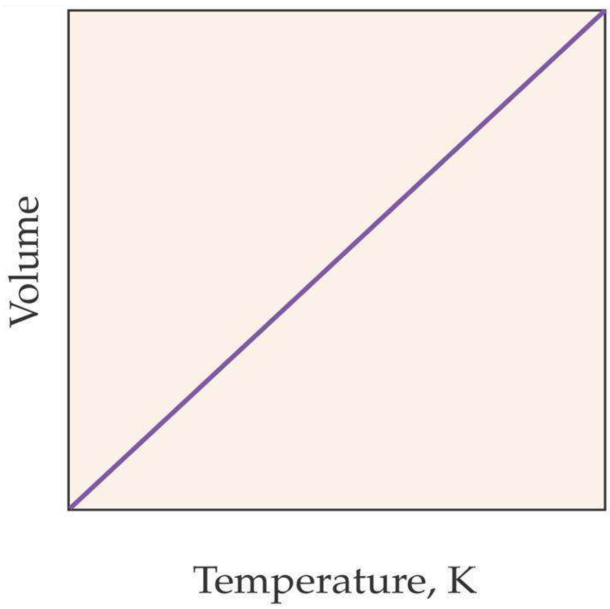
$$\frac{V_1}{T_1} = k = \frac{V_2}{T_2}$$

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$



Charles' Law





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)?

$$\frac{V_1}{T_1} = \frac{V_2}{T_2}$$

$$V_2 = V_1 \times \frac{T_2}{T_1}$$

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

Avogadro's Law

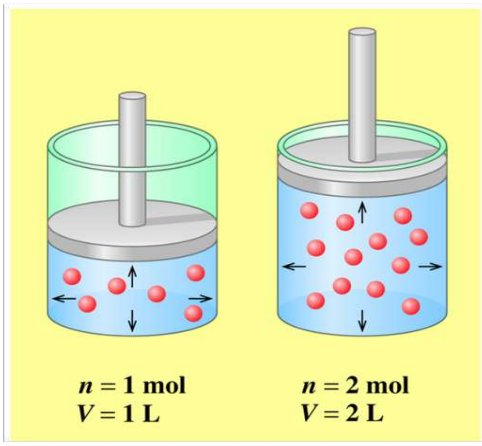
At constant pressure and temperature, volume of gas is directly proportional to the number of moles of the gas

V a number of moles (*n*)

$V = k\,n$ T and P are constant

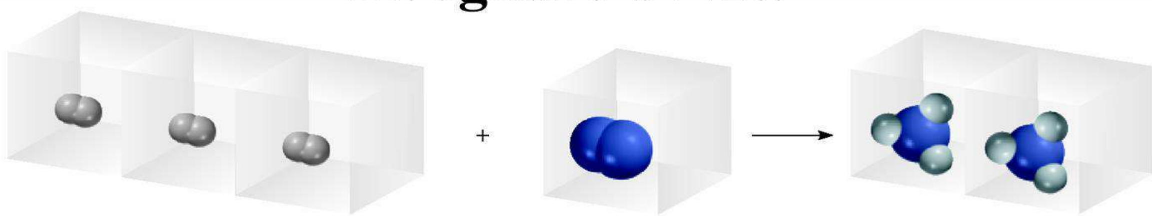
$$\frac{V}{n} = k$$

$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$



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

Avogadro's Law



$3H_2(g)$	+	$N_2(g)$	→	$2NH_3(g)$
3 molecules	+	1 molecule	→	2 molecules
3 moles	+	1 mole	→	2 moles
3 volumes	+	1 volume	→	2 volumes

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?

$$4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$$

$$1 \text{ mole } NH_3 \longrightarrow 1 \text{ mole NO}$$

At constant *T* and *P*

$$1 \text{ volume } NH_3 \longrightarrow 1 \text{ volume NO}$$

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?

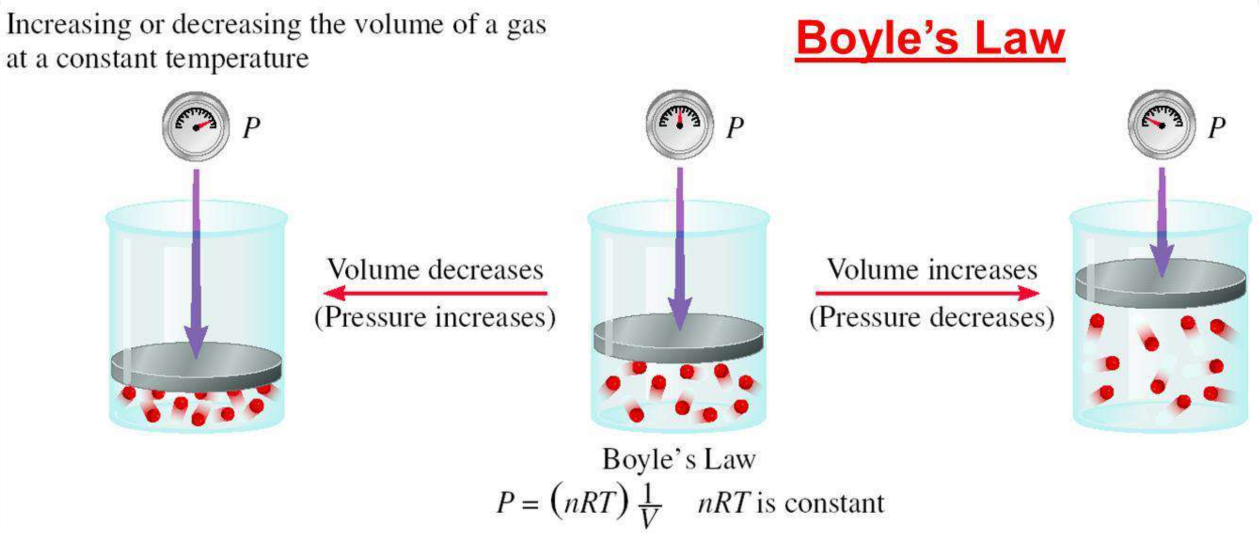
$$V_2 = V_1 \times \frac{n_2}{n_1}$$

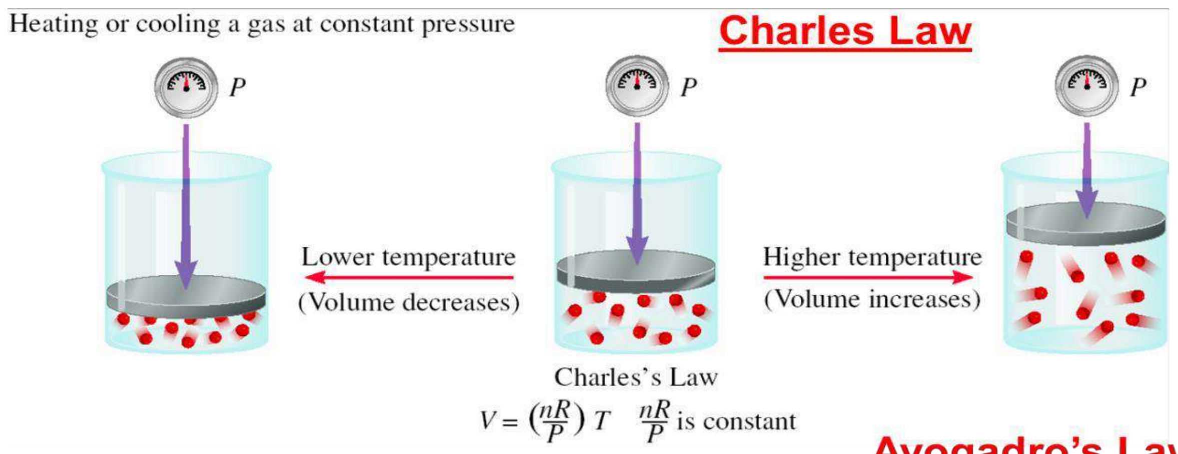
$$V_2 = 1.5 \text{ L} \times \frac{1.2 \text{ moles He}}{0.75 \text{ mole He}}$$

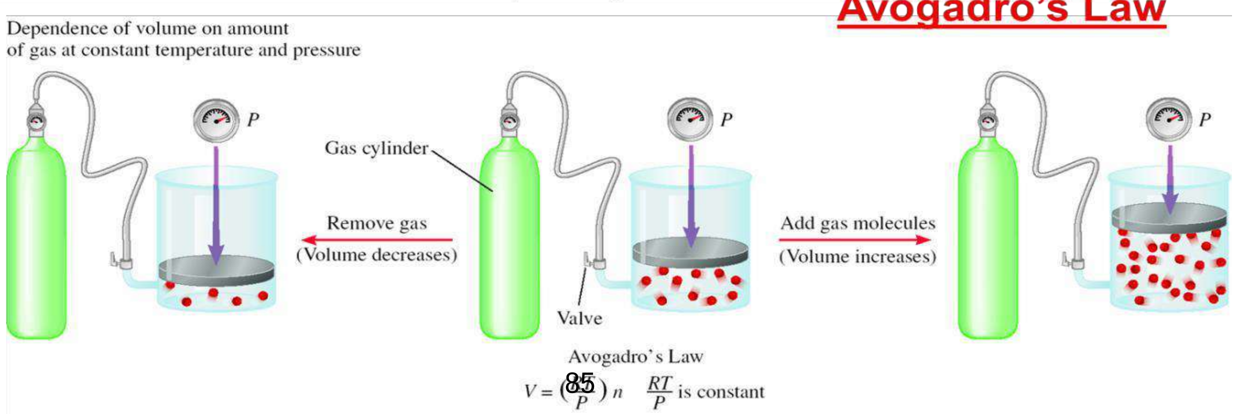
$$= 2.4\text{L}$$

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)







5.4 The Ideal Gas Equation

Ideal Gas Equation

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

Charles' law: *V* a *T* (at constant *n* and *P*)

Avogadro's law: V a *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

$$V \alpha \frac{nT}{P}$$

$$V = R\frac{nT}{P}$$

$$\boxed{PV = nRT}$$

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)

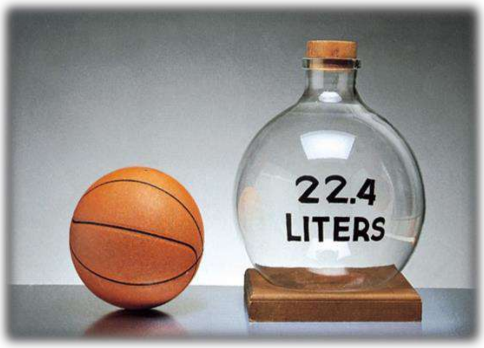
Ideal Gas

Ideal gas is a hypothetical gas whose pressure volume-temperature behaviour 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 ^{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.



$$PV = nRT$$

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

$$R = 0.082057\ \text{L} \bullet \text{atm} / (\text{mol} \bullet \text{K})$$

$$\text{R} = 0.0821 \quad \text{L} \bullet \text{atm} / (\text{mol} \bullet \text{K})$$

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

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

$P = 1\ atm$

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

$$PV = nRT$$

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

$$V = \frac{1.37\ \text{mol x } 0.0821\ \frac{\text{L•atm}}{\text{mol•K}}\text{ x } 273.15\ \text{K}}{1\ \text{atm}}$$

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

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**).

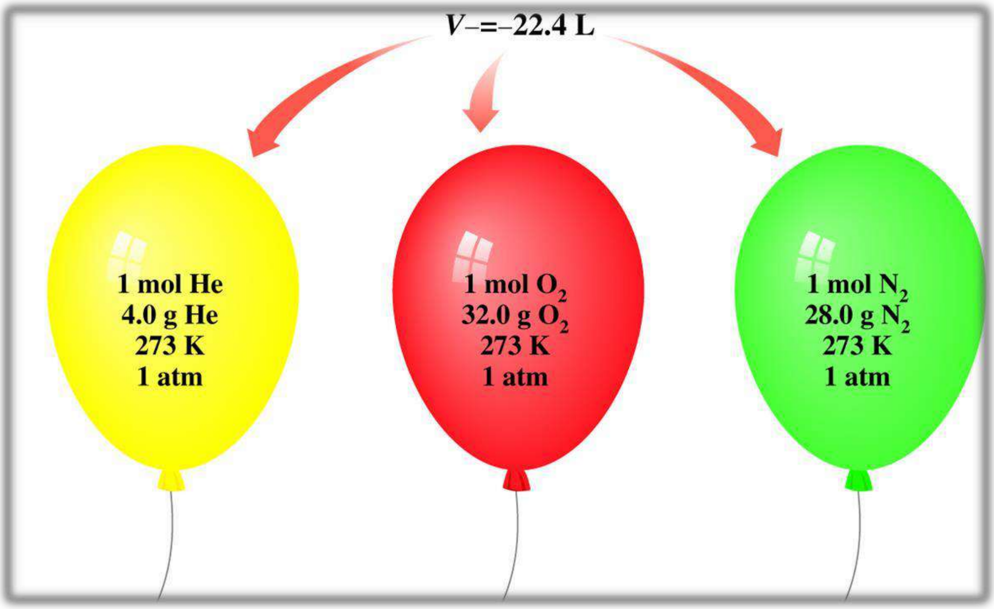
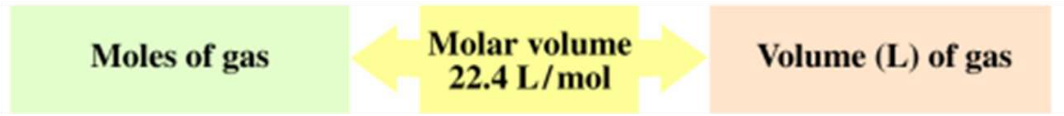


TABLE 5.1 **Volume Occupied by 1 mol of Several Different Gases at 0°C and 1 atm Pressure**

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	CO	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



What is the volume occupied by 2.75 moles N_2 gas at STP?

$$2.75 \text{ moles } N_2 \times \frac{22.41 \text{ L}}{1 \text{ mole}} = 61.63 \text{ L}$$

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

$$8.00 \text{ L} \times \frac{1 \text{ mole He}}{22.41 \text{ L}} \times \frac{4.00 \text{ g He}}{1 \text{ mole He}} = 1.43 \text{ g He}$$

Combined Gas Law

$$PV = nRT$$

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

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2}$$

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 ^{0}C is heated to 85 ^{0}C at constant volume. What is the final pressure of argon in the lightbulb (in atm)?

$PV = nRT$ $\quad$ n, V and R **are constant**

$$\frac{nR}{V} = \frac{P}{T} = \text{constant}$$

$P_1 = 1.20$ atm $\quad P_2 = ?$

$T_1 = 291$ K $\quad T_2 = 358$ K

$$\frac{P_1}{T_1} = \frac{P_2}{T_2}$$

$$P_2 = P_1 \, x \, \frac{T_2}{T_1} = 1.20 \text{ atm x } \frac{358 \cancel{K}}{291 \cancel{K}} = 1.48 \text{ atm}$$

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 K $\quad$ T_2 = -95°C + 273 = 178K

V_1 = 675 mL $\quad$ V_2 = ???

P_1 = 646 mm Hg $\quad$ P_2 = 802 mm Hg

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

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

$$V_2 = 675 \text{ mL} \times \frac{646 \text{ mm Hg} \times 178\text{K}}{802 \text{ mm Hg} \times 308\text{K}} = 314 \text{ mL}$$

Density (d) and Molar Mass (M) Calculations

$$PV = nRT$$

$$P = \frac{n}{V} RT$$

$$P = \frac{m}{\mathcal{M}} \frac{1}{V} RT$$

m is the mass of the gas in g

M is the molar mass of the gas

$$P = \frac{m}{V} \frac{1}{\mathcal{M}} RT$$

$d = \frac{m}{V}$ (in g/L)

$$P\mathcal{M} = dRT$$

$$d = \frac{P\mathcal{M}}{RT}$$

$$\mathcal{M} = \frac{dRT}{P}$$

A 2.10-L vessel contains 4.65 g of a gas at 1.00 atm and 27.0 ^{0}C. What is the molar mass of the gas?

$$\mathcal{M} = \frac{dRT}{P}$$

$$d = \frac{m}{V} = \frac{4.65\text{ g}}{2.10\text{ L}} = 2.21\,\frac{\text{g}}{\text{L}}$$

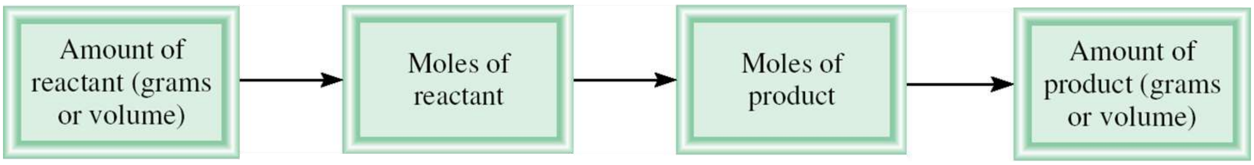
$$\mathcal{M} = \frac{2.21\,\frac{\text{g}}{\cancel{\text{L}}} \times 0.0821\,\frac{\cancel{\text{L}\bullet\text{atm}}}{\text{mol}\bullet\cancel{\text{K}}} \times 300.15\,\cancel{\text{K}}}{1\,\cancel{\text{atm}}}$$

$\mathcal{M}$ = 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?

$$4\,Al(s) + 3\,O_2\,(g) \longrightarrow 2\,Al_2O_3(s)$$

mass of Al → mole of Al → mole of O_2 → volume of O_2 (STP)

$$15.0\ g\ Al \times \frac{1\ mole\ Al}{27.0\ g\ Al} \times \frac{3\ moles\ O_2}{4\ moles\ Al} \times \frac{22.41\ L}{1\ mole\ O_2} = 9.34\ L\ O_2$$

What is the volume of CO_2 produced at 37 ^0C and 1.00 atm when 5.60 g of glucose are used up in the reaction:

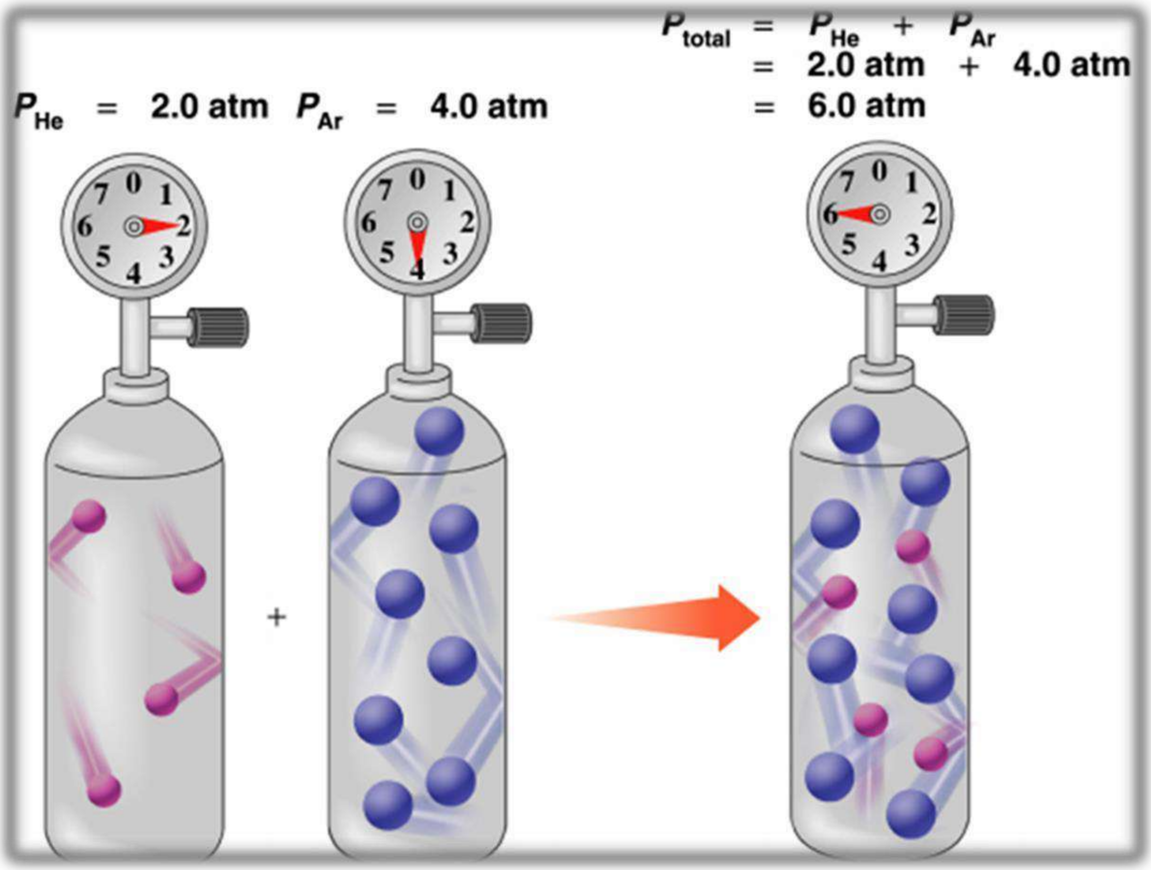
$$C_6H_{12}O_6\ (s) + 6O_2\ (g) \longrightarrow 6CO_2\ (g) + 6H_2O\ (l)$$

$$\text{g } C_6H_{12}O_6 \longrightarrow \text{mol } C_6H_{12}O_6 \longrightarrow \text{mol } CO_2 \longrightarrow V\ CO_2$$

$$5.60 \text{ g } C_6H_{12}O_6 \times \frac{1 \text{ mol } C_6H_{12}O_6}{180 \text{ g } C_6H_{12}O_6} \times \frac{6 \text{ mol } CO_2}{1 \text{ mol } C_6H_{12}O_6} = 0.187 \text{ mol } CO_2$$

$$V = \frac{nRT}{P} = \frac{0.187 \text{ mol} \times 0.0821 \frac{\text{L•atm}}{\text{mol•K}} \times 310.15 \text{ K}}{1.00 \text{ atm}} = 4.76 \text{ L}$$

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.

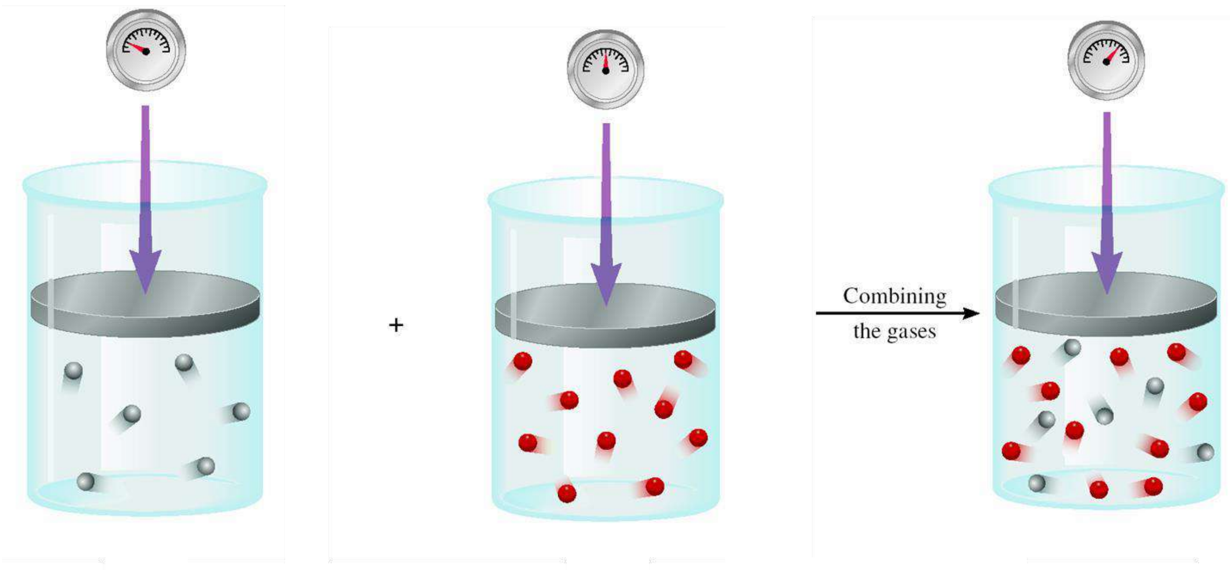
Dalton's Law of Partial Pressures states that the total pressure of a gaseous mixture is equal to the sum of the individual pressures of each gas.

$$P1 + P2 + P3 + \ldots = P\ total$$

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

Dalton's Law of Partial Pressures

V and *T* are **constant**



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

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_2O	5.7	
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?

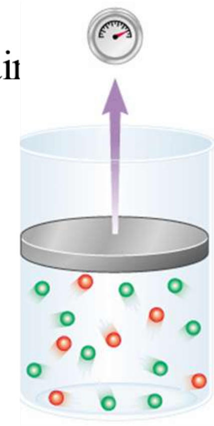
$$0.450 \text{ atm} \times \frac{760 \text{ mm Hg}}{1 \text{ atm}} = 342 \text{ mm Hg} = P_{O_2}$$

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

$$P_{\text{total}} = 342 \text{ mm Hg} + 855 \text{ mm Hg}$$

$$= 1197 \text{ mm Hg}$$

Consider a case in which two gases, A and B, are in a contai volume V.



$$P_A = \frac{n_A RT}{V}$$ n_A is the number of moles of A

$$P_B = \frac{n_B RT}{V}$$ n_B is the number of moles of B

$$P_T = P_A + P_B \qquad X_A = \frac{n_A}{n_A + n_B} \qquad X_B = \frac{n_B}{n_A + n_B}$$

$$P_A = X_A P_T \qquad P_B = X_B P_T$$

$$\boxed{P_i = X_i P_T}$$

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

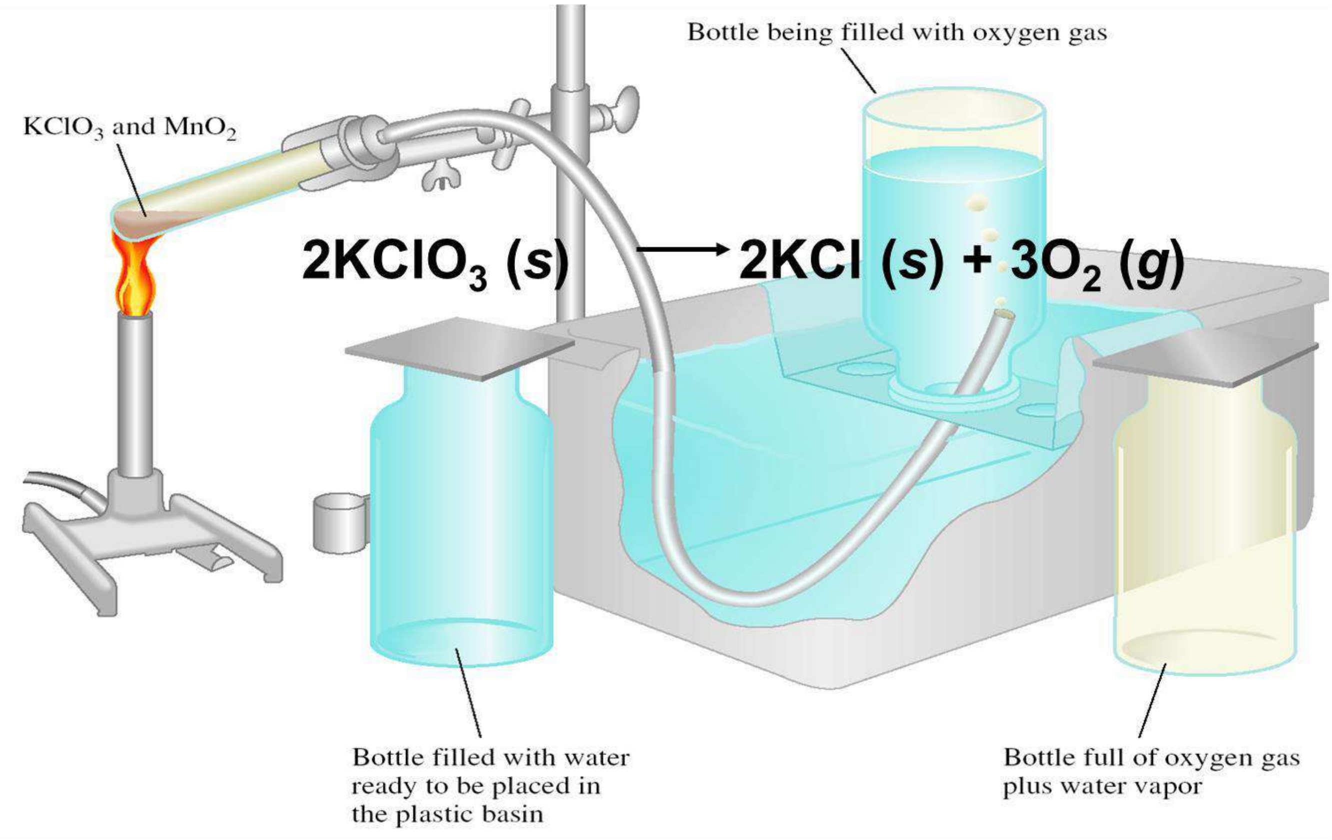
A sample of natural gas contains 8.24 moles of CH_4, 0.421 moles of C_2H_6, and 0.116 moles of C_3H_8. If the total pressure of the gases is 1.37 atm, what is the partial pressure of propane (C_3H_8)?

$$P_i = X_i P_T \qquad P_T = 1.37 \text{ atm}$$

$$X_{propane} = \frac{0.116}{8.24 + 0.421 + 0.116} = 0.0132$$

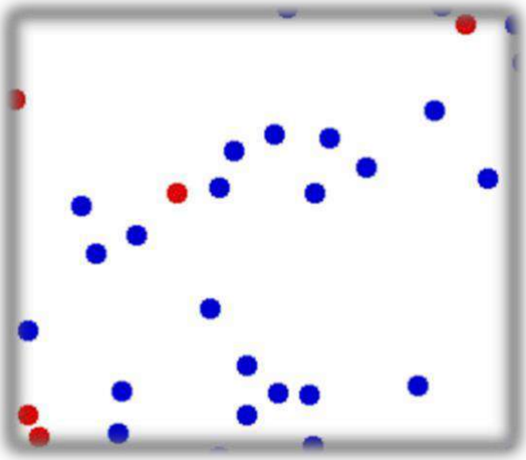
$$P_{propane} = 0.0132 \times 1.37 \text{ atm} = 0.0181 \text{ atm}$$

Collecting a Gas over Water



$$P_T = P_{O_2} + P_{H_2O}$$

5.7 Kinetic Molecular Theory of Gases



Kinetic Molecular Theory of Gases

This theory explains the behavior of gases

1. 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

$\overline{KE} = \frac{1}{2} m\overline{u^2}$ — m = *mass of the molecule*

$\overline{KE} \propto T$ — $\overline{u^2}$ = *mean square speed*

$\frac{1}{2} m\overline{u^2} \propto T$ — C = *proportionality constant*

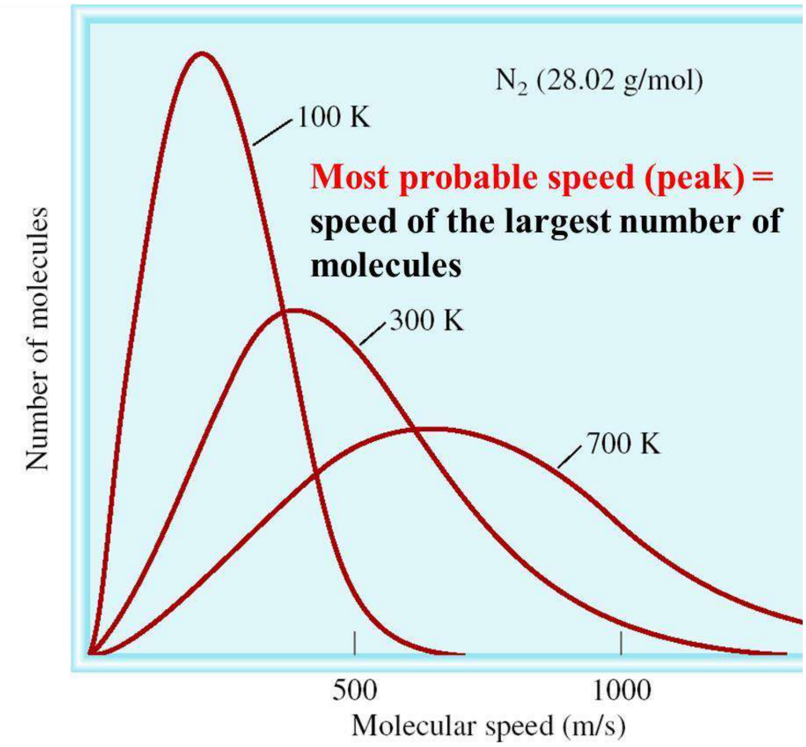
$\frac{1}{2} m\overline{u^2} = CT$

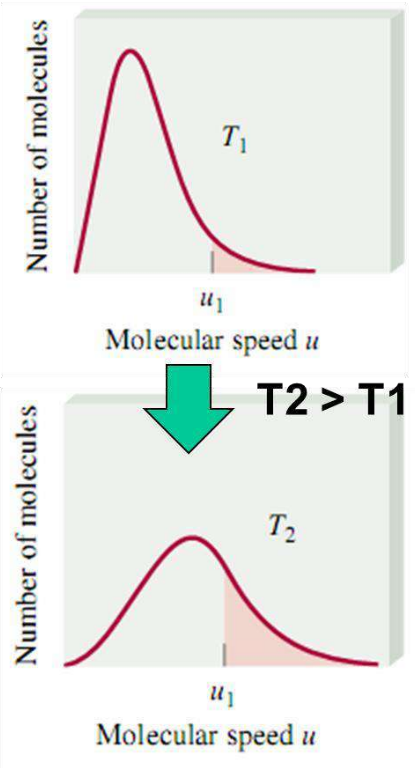
∴ The T of a gas is a measure of the average KE of the molecules

Maxwell speed distribution curves

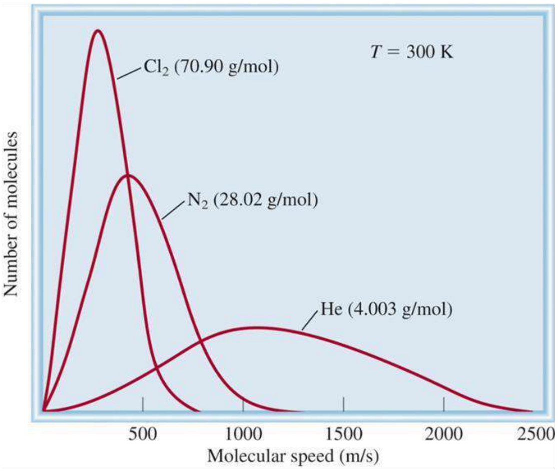
The distribution of gas molecule speeds at various temperature

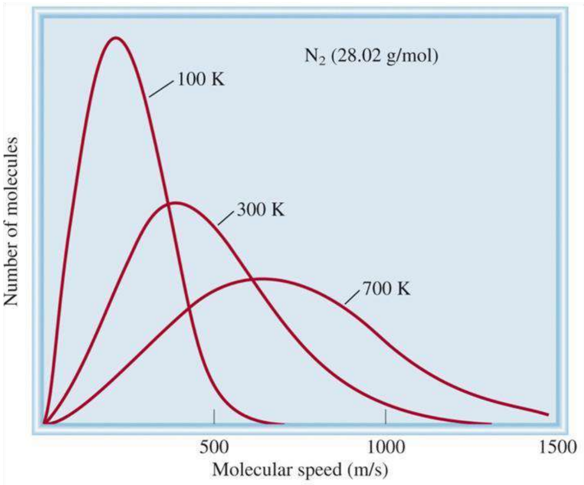
↑T, ↑ number of molecules moving at high speed





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





Average molecular speed of a gas

$$u_{rms} = \sqrt{\frac{3RT}{\mathcal{M}}}$$

Unit = m/s

T in K

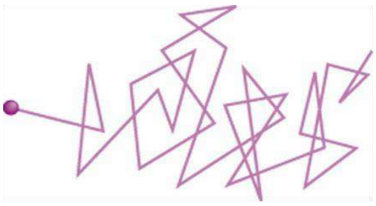
$\mathcal{M}$ in kg/mol

R = 8.314 J/K. mol

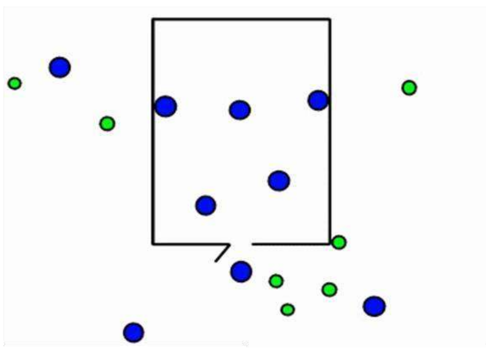
$1\ J = 1\ kg\ m^2/s^2$

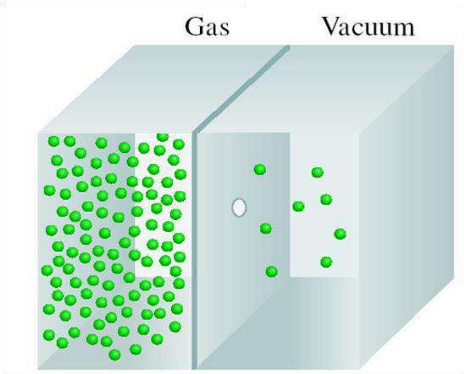
u_{rms} of smaller mass (lighter) gas > u_{rms} of higher mass (heavier) gas

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



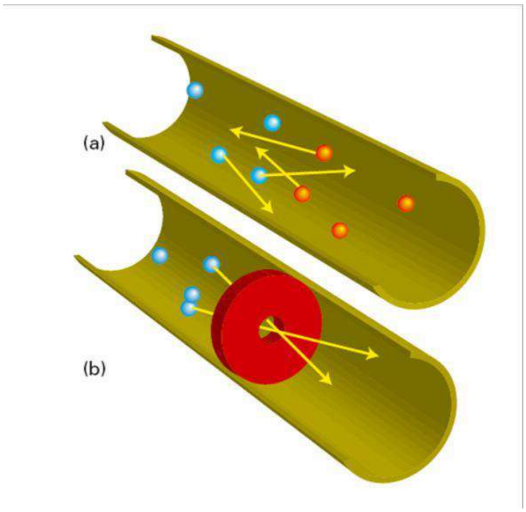
molecular path

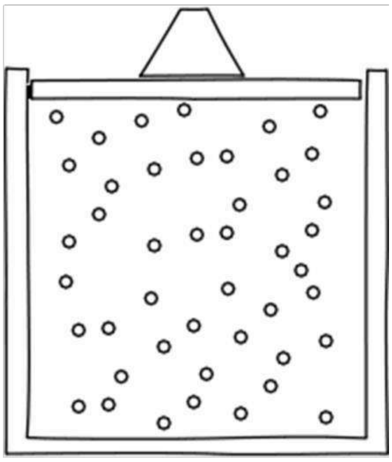


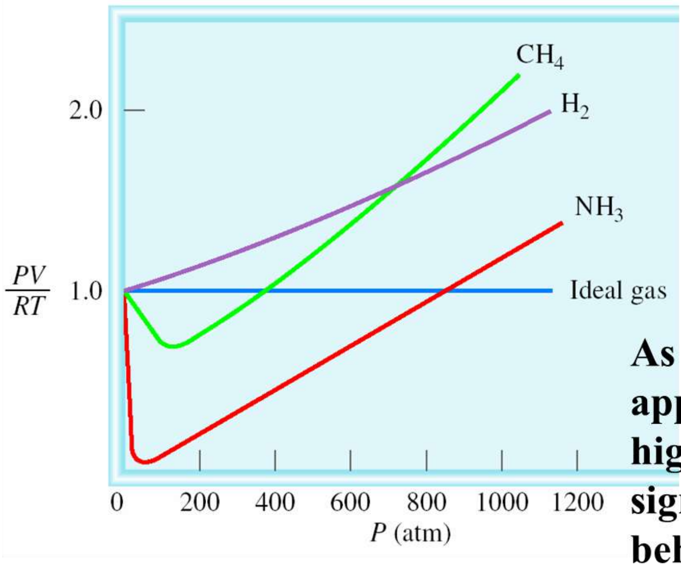


Gas effusion is the is the process by which gas under pressure escapes from one compartment of a container to another by passing through a small opening.

5.8 Deviations from Ideal Behaviour





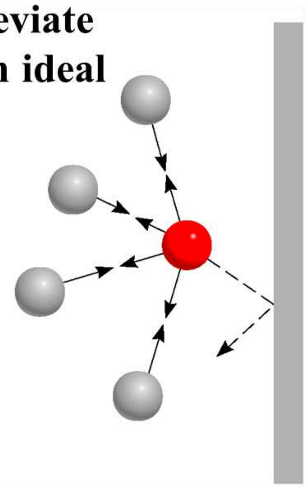


1 mole of ideal gas

$$PV = nRT$$

$$n = \frac{PV}{RT} = 1.0$$

As P approaches zero, all gases approach ideal behavior. At higher P, gases deviate significantly from ideal behavior

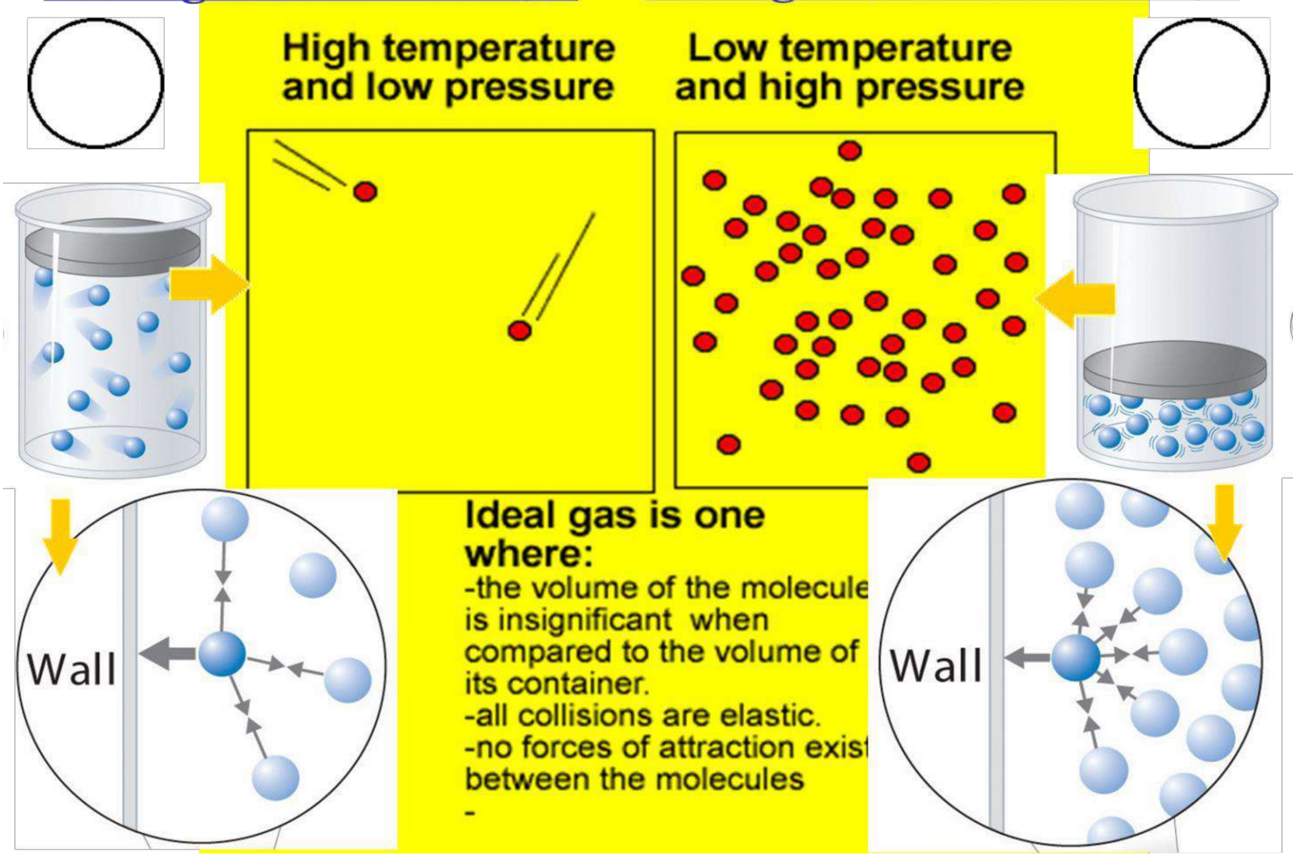


Why real gases deviate from ideal behavior ???

At higher P, gas density ↑, 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

$$\underbrace{\left(P + \frac{an^2}{V^2}\right)}_{\text{corrected pressure}}\underbrace{(V - nb)}_{\text{corrected volume}} = nRT$$

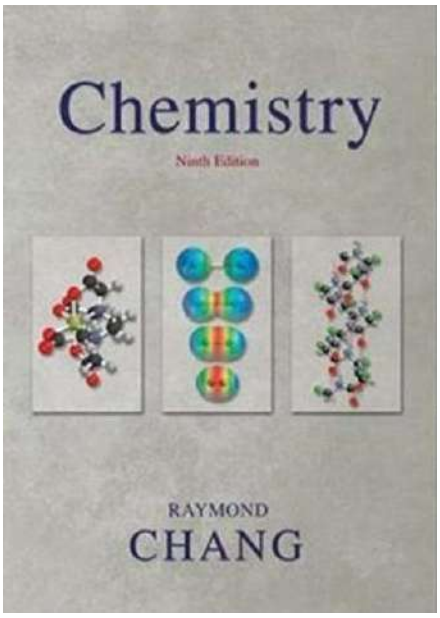
a, b = constant

TABLE 5.4
van der Waals Constants of Some Common Gases

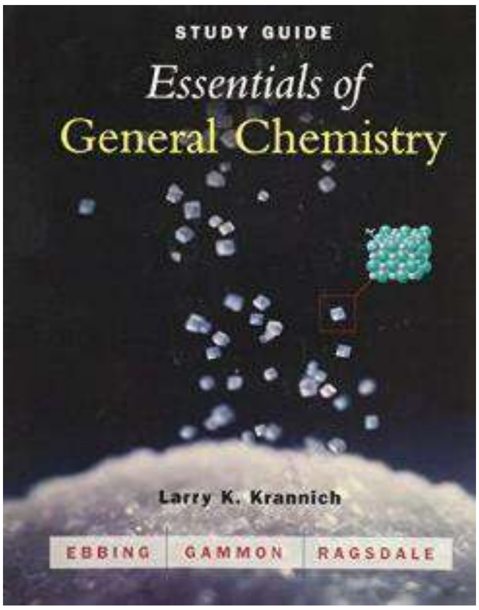
Gas	a $\left(\frac{atm \cdot L^2}{mol^2}\right)$	b $\left(\frac{L}{mol}\right)$
He	0.034	0.0237
Ne	0.211	0.0171
Ar	1.34	0.0322
Kr	2.32	0.0398
Xe	4.19	0.0266
H_2	0.244	0.0266
N_2	1.39	0.0391
O_2	1.36	0.0318
Cl_2	6.49	0.0562
CO_2	3.59	0.0427
CH_4	2.25	0.0428
CCl_4	20.4	0.138
NH_3	4.17	0.0371
H_2O	5.46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

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.



2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 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

6.5 Calorimetry

6.6 Standard Enthalpy of Formation and Reaction

6.7 Heat of Solution and dilution

6.1 The nature of energy and types of energy

Energy is the capacity to do work.

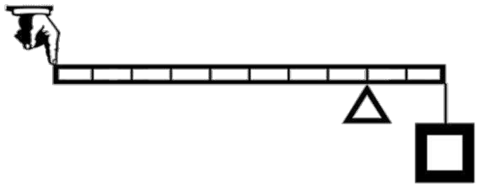
Work(w) = energy used to move an object over some distance

= force x distance (F x *d*)

= 1 kgm^2/s^2

= 1 Nm

= 1 J



SI 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/s^2)

Force = mass (kg) x acceleration (m/s^2)

= kgm/s^2

= N

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

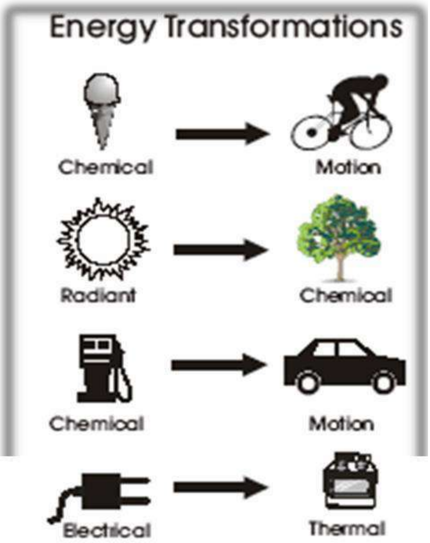
•***Chemical energy*** is the energy stored within the bonds of chemical substances

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

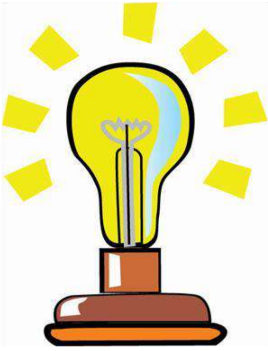
6.2 Energy changes in chemical reactions

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



electrical energy to light energy to thermal and radiant energy

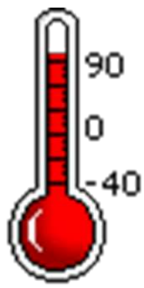
Potential energy to kinetic energy

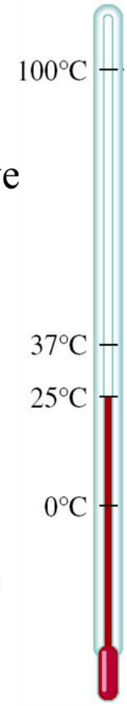
Almost all chemical reactions absorb/produce energy in the form of heat

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

Temperature is a measure of the thermal energy.

Temperature ≠ Thermal Energy

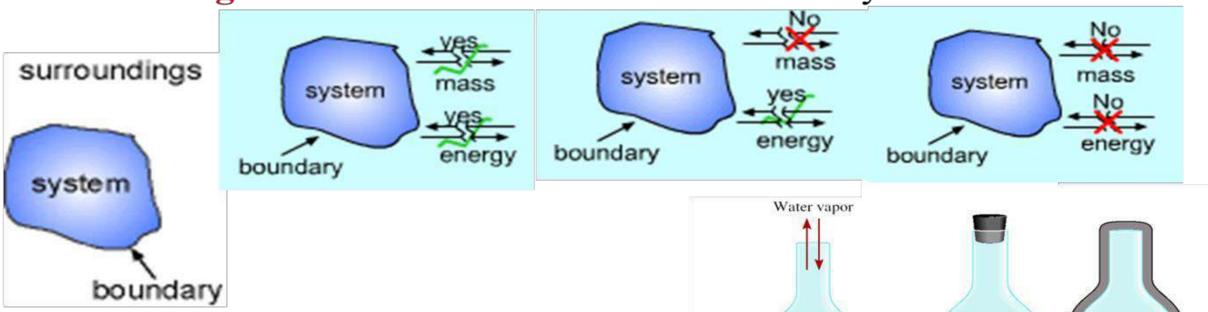




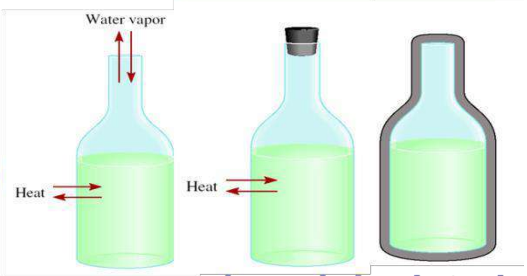
System and Surroundings

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.



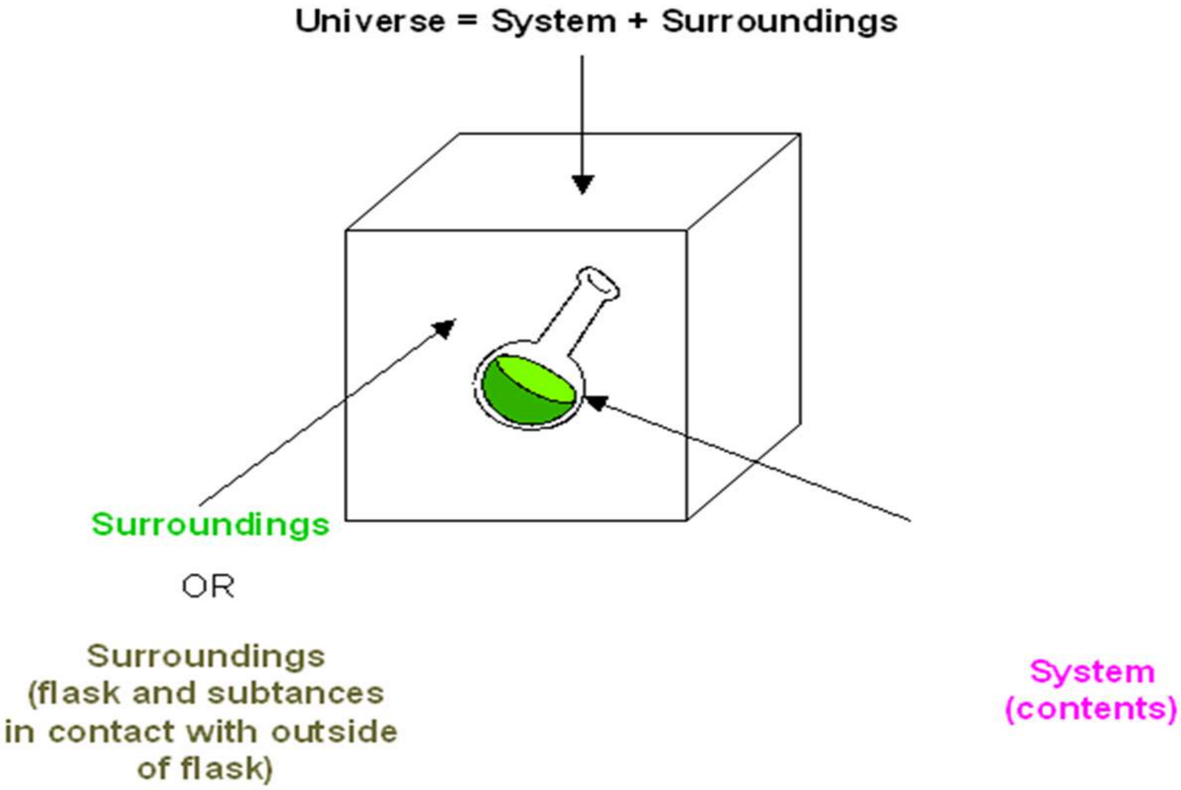
In chemical reactions, energy (heat) is often transferred from the "system" to its "surroundings," or vice versa.



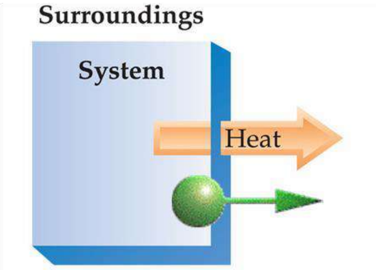
open **closed** **isolated**

Exchange: mass & energy energy nothing

System and Surrounding



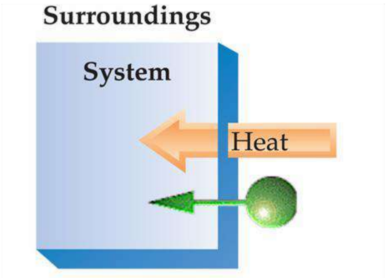
Exothermic process is any process that gives off heat – transfers thermal energy from the system to the surroundings.



$$2H_2\,(g) + O_2\,(g) \longrightarrow 2H_2O\,(l) + \text{energy}$$

$$H_2O\,(g) \longrightarrow H_2O\,(l) + \text{energy}$$

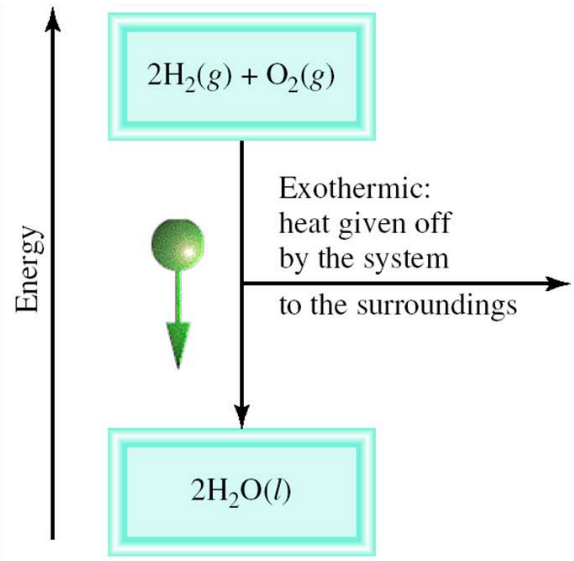
Endothermic process is any process in which heat has to be supplied to the system from the surroundings.



$$\text{energy} + 2HgO\,(s) \longrightarrow 2Hg\,(l) + O_2\,(g)$$

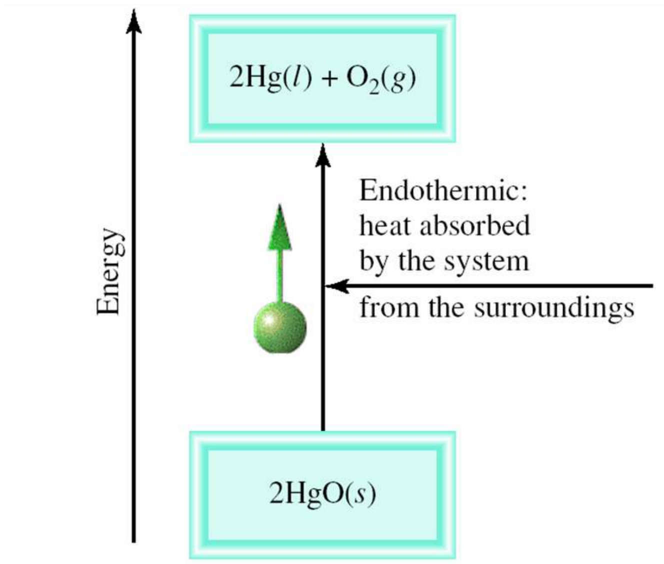
$$\text{energy} + H_2O\,(s) \longrightarrow H_2O\,(l)$$

Exothermic



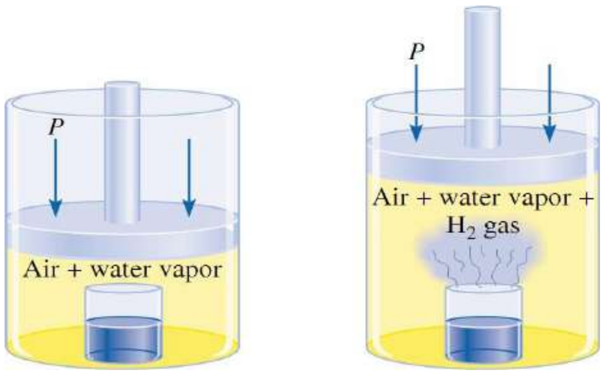
energy of the products < energy of the reactants

Endothermic



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.

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

$\Delta P = P_{final} - P_{initial}$ $\Delta T = T_{final} - T_{initial}$ $\Delta w \neq w_{final} - w_{initial}$

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

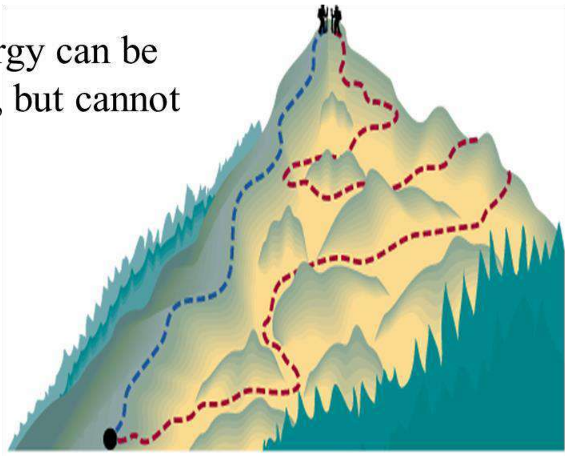
$\Delta q \neq q_{final} - q_{initial}$

- **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.



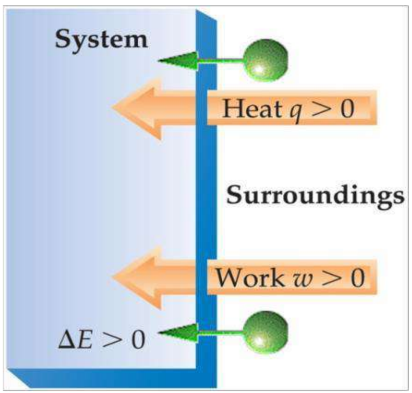
First law of thermodynamics – energy can be converted from one form to another, but cannot be created or destroyed.

Change in internal energy,
$DE = E_{final} - E_{initial}$
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

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

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



Change of energy (DE)

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

DE = q + w

DE = the change in internal energy of a system

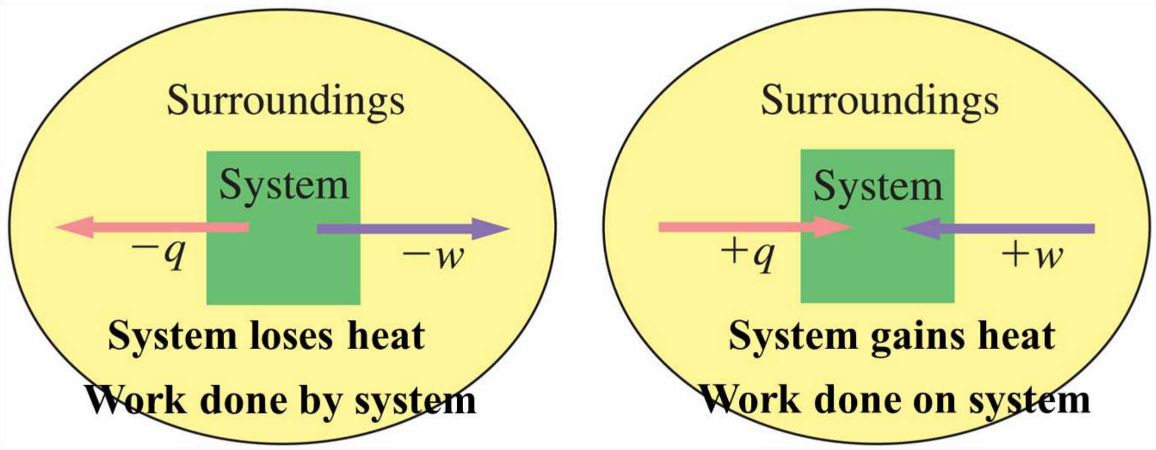
q = the heat exchange between the system and the surroundings

w = the work done on (or by) the system

Sign conventions for work & heat

$\Delta E = q + w$

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)	−



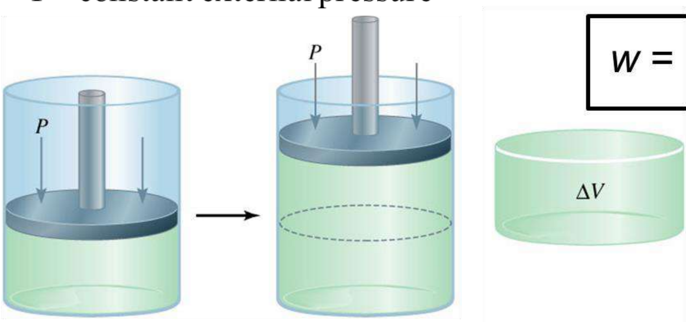
- DE (loss of internal energy) **+ DE (gain of internal energy)**

Work and Heat

$w = F \times d$ unit = J

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

P= constant external pressure

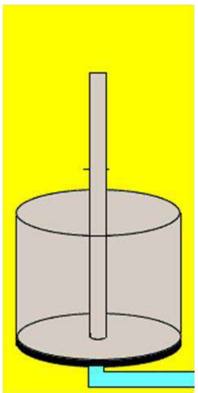


$w = -P\,\Delta V$ unit = L . atm

1 L . atm = 101.3 J

$$P \times V = \frac{F}{d^2} \times d^3 = F \times d = w$$

Gas compression	Gas expansion
Work done on the system by the surrounding	Work done by the system to the surrounding
Vf-Vi < 0	Vf-Vi > 0
DV < 0	*DV > 0*
∴ w is positive	∴ w is negative

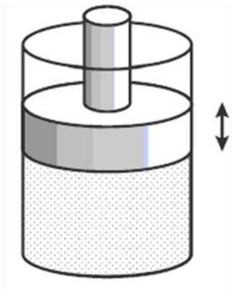


A sample of nitrogen gas expands in volume from 1.6 L to 5.4 L at constant temperature. What is the work done in joules if the gas expands (a) against a vacuum and (b) against a constant pressure of 3.7 atm?

$$w = -P\,\Delta V$$

(a) ΔV = 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) ΔV = 5.4 L – 1.6 L = 3.8 L P = 3.7 atm

w = -3.7 atm x 3.8 L = -14.1 L•atm

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

(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

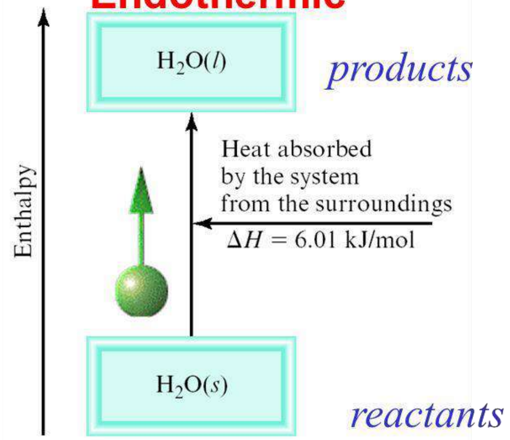
$$H = E + PV$$

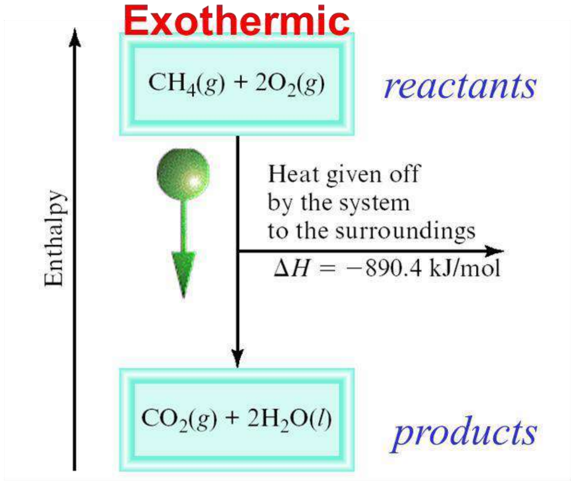
$DH = DE + PDV$	P constant
$DH = (q+w)$ -w	$DE = q + w$
$DH = q$	$w = -P\,DV$

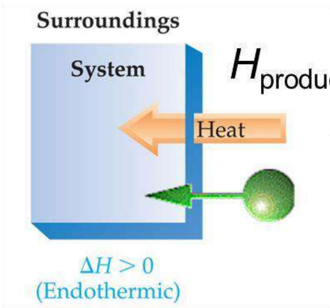
Change of enthalpy of the system = heat flow into/out the system (heat gain/heat lost)

Enthalpy of reaction, D*H* = *H* (products) – *H* (reactants)

Endothermic **Exothermic**

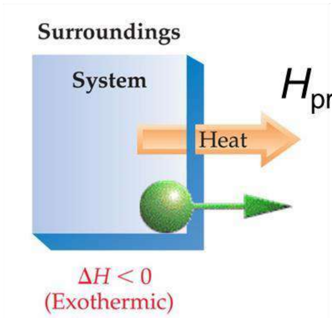






$H_{products} > H_{reactants}$

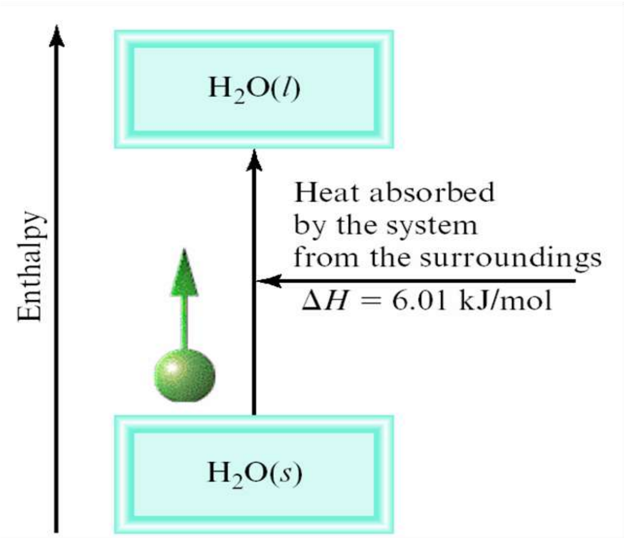
$\Delta H > 0$



$H_{products} < H_{reactants}$

$\Delta H < 0$

Thermochemical Equations



Is ΔH negative or positive?

System absorbs heat

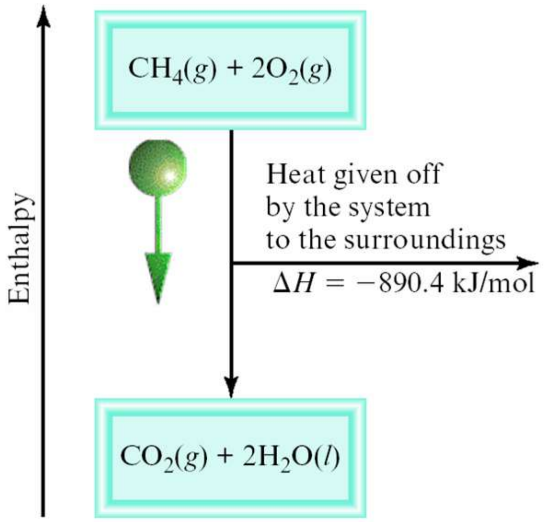
Endothermic

$\Delta H > 0$

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

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

Thermochemical Equations



Is ΔH negative or positive?

System gives off heat

Exothermic

$\Delta H < 0$

890.4 kJ are released for every 1 mole of methane that is combusted at 25^0C and 1 atm.

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

Thermochemical Equations

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

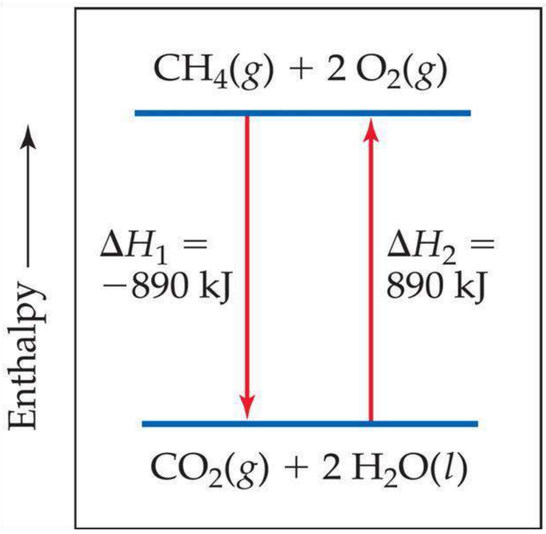
$$H_2O\ (s) \longrightarrow H_2O\ (l)$$

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

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

$$H_2O\ (l) \longrightarrow H_2O\ (s)$$

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



Thermochemical Equations

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

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

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

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

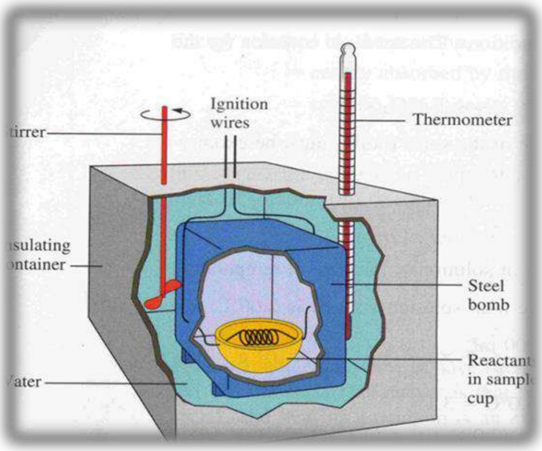
$$H_2O\ (l) \longrightarrow H_2O\ (g) \quad \Delta H = 44.0\ \text{kJ/mol}$$

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

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

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

6.5 Calorimetry



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 substance by **one degree** Celsius.

Unit = J/g · °C

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/°C

$$C = ms$$

Heat (*q*) absorbed or released:

$$q = C\Delta t$$

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

$$q = ms\Delta t$$

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

Substance	Specific Heat (J/g · °C)
Al	0.900
Au	0.129
C (graphite)	0.720
C (diamond)	0.502
Cu	0.385
Fe	0.444
Hg	0.139
H_2O	4.184
C_2H_5OH (ethanol)	2.46

Determine the heat capacity for 60.0g of water.

$$C = ms$$
$$= (60.0g)(4.184\ J/g \cdot {}^oC)$$
$$= 251\ J/{}^oC$$

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

$$q = ms\Delta t$$

$$q = (466g)(4.184\ J/g \cdot {}^oC)(74.60\ {}^oC - 8.50\ {}^oC)$$

$$q = 128878\ J$$

$$q = 129\ kJ$$

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

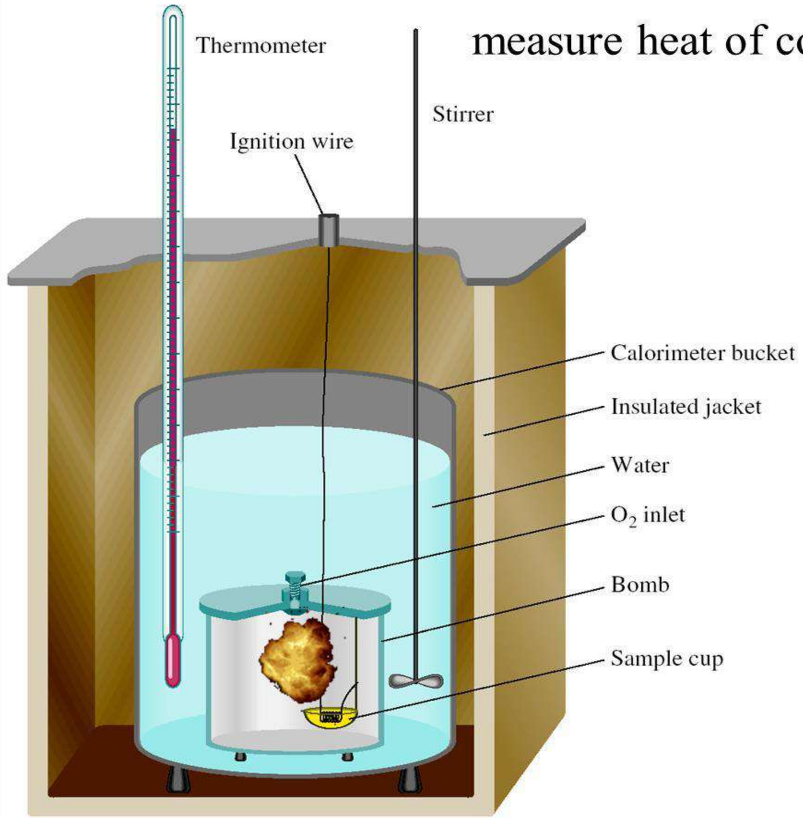
s of Fe = 0.444 J/g • ^oC

$$\Delta t = t_{final} - t_{initial}$$
$$= 5^oC - 94^oC = -89^oC$$

$$q = ms\Delta t$$
$$= 869\ g \times 0.444\ J/g \cdot {}^oC \times -89^oC$$
$$= -34{,}000\ J$$
$$= -34\ kJ$$

Constant-Volume Calorimetry ("Bomb" calorimeter)

measure heat of combustion



$q_{rxn} = -(q_{water} + q_{cal})$

$q_{water} = ms\Delta t$

$q_{cal} = C_{cal}\,\Delta t$

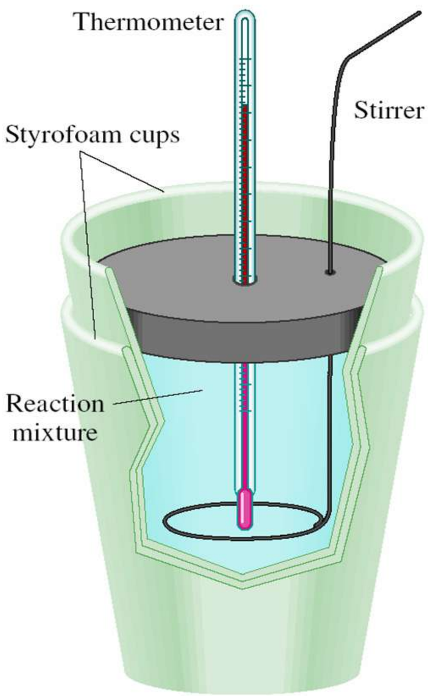
Reaction at Constant V

$\Delta H \neq q_{rxn}$

$\Delta H \approx q_{rxn}$

No heat/mass enters/leaves (isolated system)

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



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

$\Delta H = q_{rxn}$

No heat enters or leaves!

TABLE 6.3	Heats of Some Typical Reactions Measured at Constant Pressure	
Type of Reaction	**Example**	**ΔH (kJ/mol)**
Heat of neutralization	$HCl(aq) + NaOH(aq) \longrightarrow NaCl(aq) + H_2O(l)$	−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…

$$q_{rxn} = -(q_{water} + q_{calorimeter})$$

Heat lost = exothermic (↑ q_{rxn})

Heat gained = endothermic (↑ $q_{water} + q_{calorimeter}$)

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

$$q = -(q_{water} + q_{cal})$$

$q_{water} = ms\Delta t$

$= (2000g)(4.184 J/g.\,^{\circ}C)(25.84\,^{\circ}C - 20.17\,^{\circ}C)$

$= 47400$ J or 47.4 kJ

$q_{bomb} = C\Delta t$

$= (1.80\ kJ/^{\circ}C)(25.84\,^{\circ}C - 20.17\,^{\circ}C)$

$= 10.2$ kJ

$q = -(q_{water} + q_{cal})$

$q = -(47.4\ kJ + 10.2\ kJ) = -57.6\ kJ$

6.6 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 **(DH^0)** is$_f$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.

$\Delta H^0_f(O_2) = 0$
$\Delta H^0_f(O_3) = 142$ kJ/mol
ΔH^0_f (C, graphite) = 0
ΔH^0_f (C, diamond) = 1.90 kJ/mol

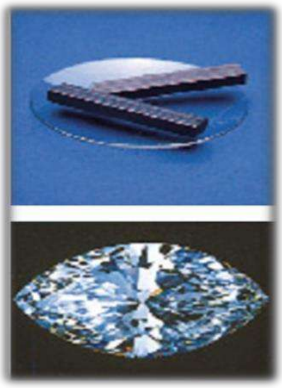


TABLE 6.4 Standard Enthalpies of Formation of Some Inorganic Substances at 25°C

Substance	ΔH_f°(kJ/mol)	Substance	ΔH_f°(kJ/mol)
$Ag(s)$	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
$Br_2(l)$	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
$Cl_2(g)$	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^0_{rxn}) is the enthalpy of a reaction carried out at 1 atm.

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

$$\Delta H^0_{rxn} = [c\Delta H^0_f(C) + d\Delta H^0_f(D)] - [a\Delta H^0_f(A) + b\Delta H^0_f(B)]$$

$$\Delta H^0_{rxn} = \Sigma n\Delta H^0_f\text{(products)} - \Sigma m\Delta H^0_f\text{(reactants)}$$

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.

$$CaO(s) + CO_2(g) \longrightarrow CaCO_3(s) \qquad \Delta H^o_{rxn} = -177.8\ kJ/mol$$

$$\Delta H^o_{rxn} = \Sigma n\Delta H^o_f(products) - \Sigma n\Delta H^o_f(reactants)$$

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

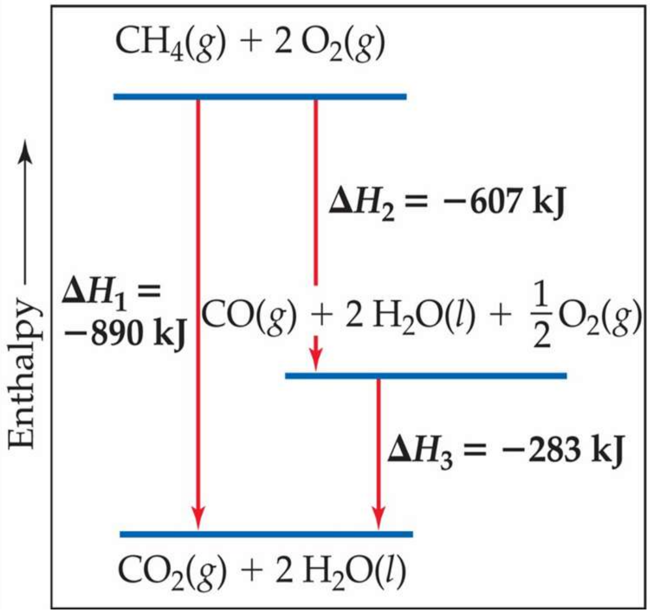
$$\Delta H_f^o \text{ for } CaO(s) = -635.6\ kJ$$

The Indirect Method for Determining ΔH^0

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

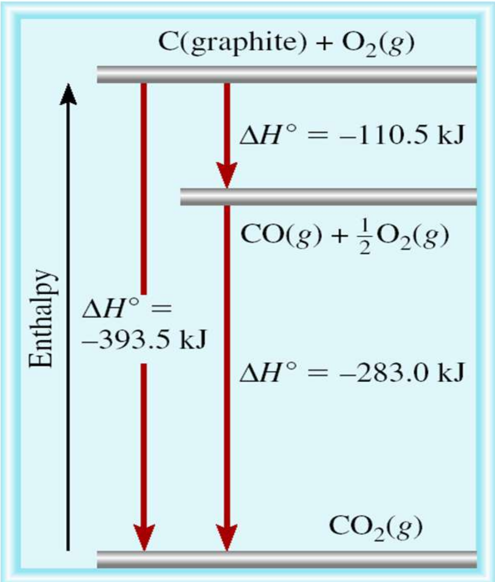
Hess's Law: When reactants are converted to products, the change in enthalpy is the same whether the reaction takes place in one step or in a series of steps.

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.



$$C\,(graphite) + 1/2O_2\,(g) \longrightarrow CO\,(g)$$
$$CO\,(g) + 1/2O_2\,(g) \longrightarrow CO_2\,(g)$$
$$\overline{C\,(graphite) + O_2\,(g) \longrightarrow CO_2\,(g)}$$

Indirect method (Hess's Law)

$$S(s) + O_2(g) \rightarrow SO_2(g);\;\; \Delta H^o = \text{-}297\,kJ$$

$$2SO_3(g) \rightarrow 2SO_2(g) + O_2(g);\;\; \Delta H^o = 198\,kJ$$

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

Answer :

$$2S(s) + 2O_2(g) \rightarrow \cancel{2SO_2}(g);\;\; \Delta H^o = (\text{-}297\,kJ) \times (2)$$

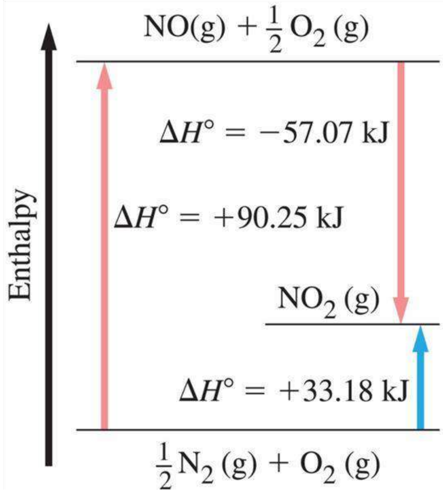
$$\cancel{2SO_2}(g) + O_2(g) \rightarrow 2SO_3(g);\;\; \Delta H^o = (198\,kJ) \times (\text{-}1)$$

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

$$NO(g) \rightarrow \tfrac{1}{2}N_2(g) + \tfrac{1}{2}O_2(g) \quad \Delta H = -90.25\ kJ$$
$$NO(g) + \tfrac{1}{2}O_2(g) \rightarrow NO_2(g) \quad \Delta H = -57.07\ kJ$$
$$\tfrac{1}{2}N_2(g) + O_2(g) \rightarrow NO_2(g) \quad \Delta H = ??$$

$$\tfrac{1}{2}N_2(g) + \tfrac{1}{2}O_2(g) \rightarrow NO(g) \quad \Delta H = +90.25\ kJ$$
$$NO(g) + \tfrac{1}{2}O_2(g) \rightarrow NO_2(g) \quad \Delta H = -57.07\ kJ$$

$$\tfrac{1}{2}N_2(g) + O_2(g) \rightarrow NO_2(g) \quad \Delta H = +33.18\ kJ$$



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.

$$2C_6H_6(l) + 15O_2(g) \longrightarrow 12CO_2(g) + 6H_2O(l)$$

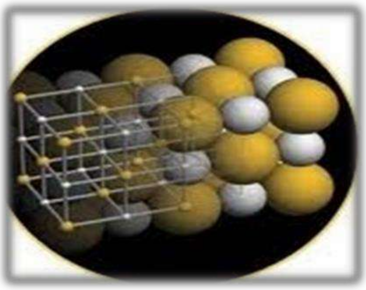
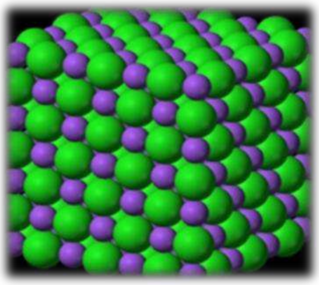
$$\Delta H^0_{rxn} = \Sigma n\Delta H^0_f\,(\text{products}) - \Sigma m\Delta H^0_f\,(\text{reactants})$$

$$\Delta H^0_{rxn} = [12\Delta H^0_f\,(CO_2) + 6\Delta H^0_f\,(H_2O)] - [2\Delta H^0_f\,(C_6H_6)]$$

$$\Delta H^0_{rxn} = [\,12\text{x}-393.5 + 6\text{x}-187.6\,] - [\,2\text{x}49.04\,] = -5946\ kJ$$

$$\frac{-5946\ kJ}{2\ mol} = -2973\ kJ/mol\ C_6H_6$$

6.7 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**.

$$DH_{soln} = H_{soln} - H_{components}$$

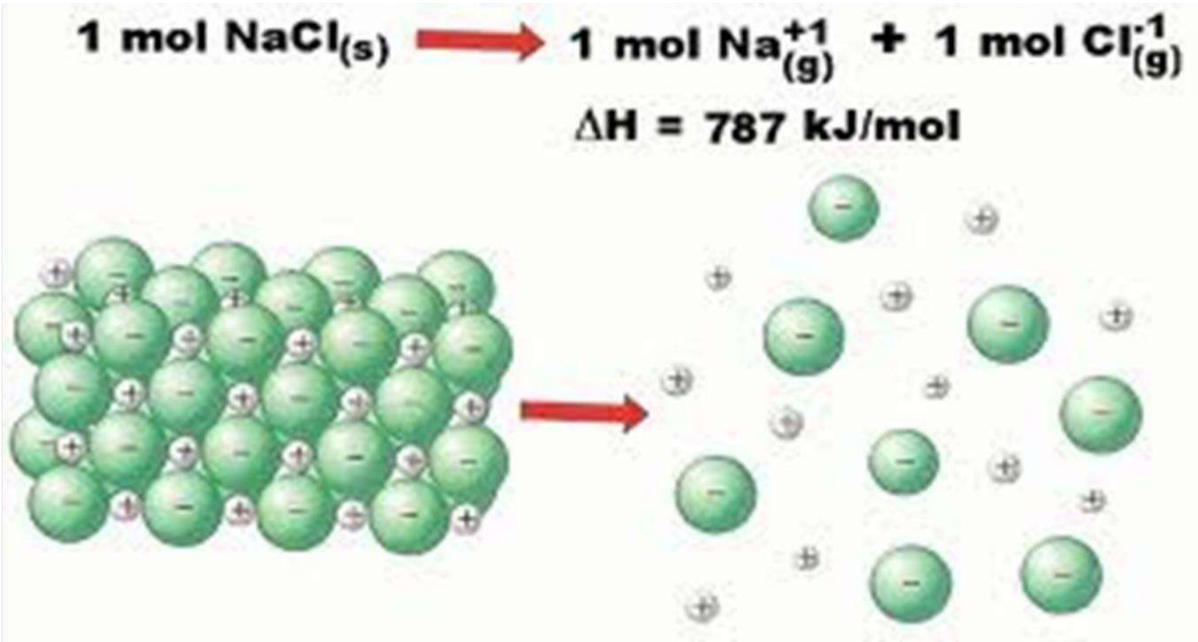
The ***heat of dilution*** is the **heat change** associated with the **dilution** process.

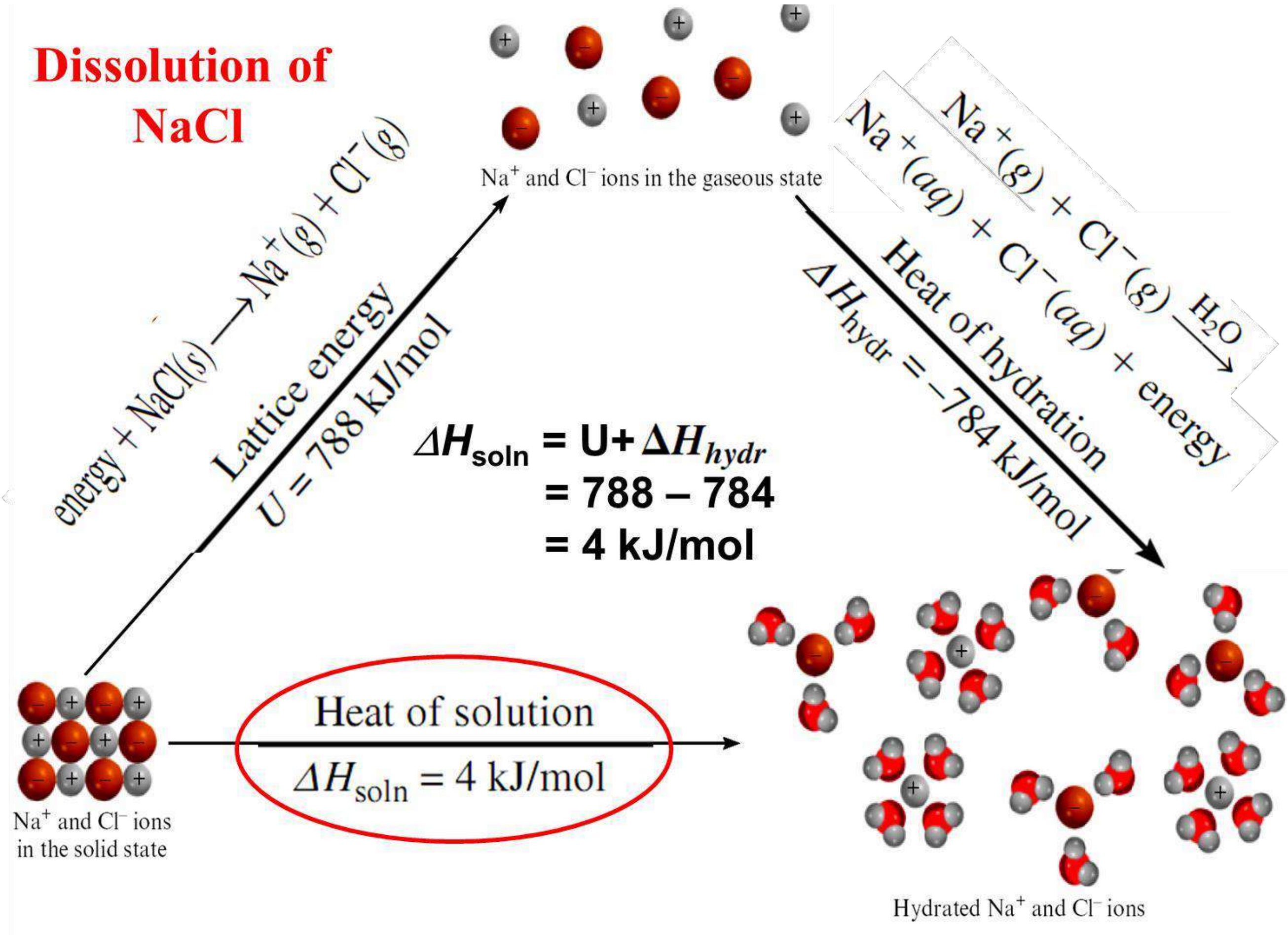
Heats of Solution of Some Ionic Compounds	
Compound	**ΔH_{soln} (kJ/mol)**
LiCl	−37.1
$CaCl_2$	−82.8
NaCl	4.0
KCl	17.2
NH_4Cl	15.2
NH_4NO_3	26.2

Lattice energy (U) = the energy required to completely separate **one mole** of a **solid** ioniccompound into **gaseous** ions

Heat of hydration (ΔH_{hydr} **=** the enthalpy change associated with the **hydration** process

Lattice energy (U)





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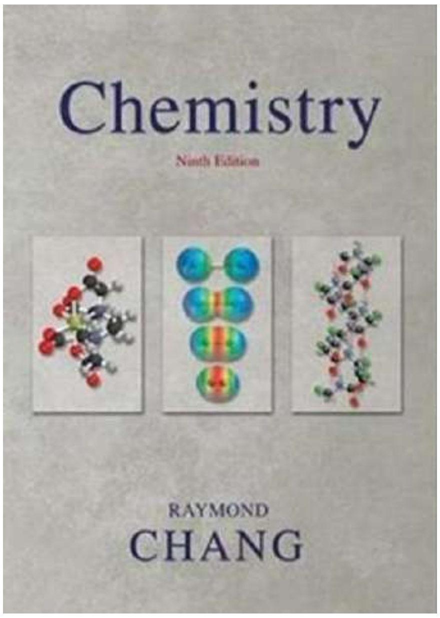

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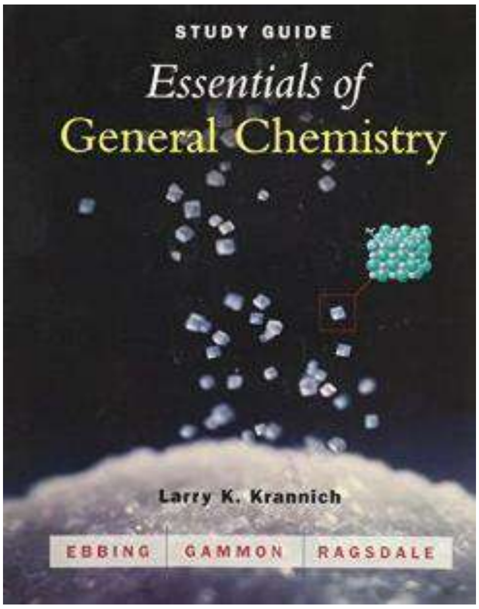
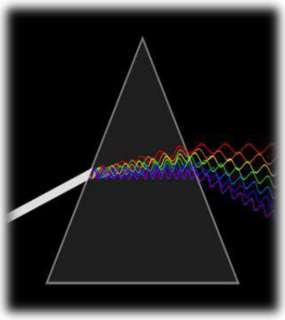


LECTURE 7

Quantum Theory and The Electronic Structure of Atoms





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

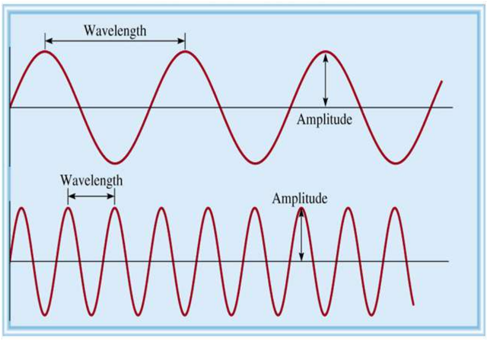
7.5 Quantum Numbers

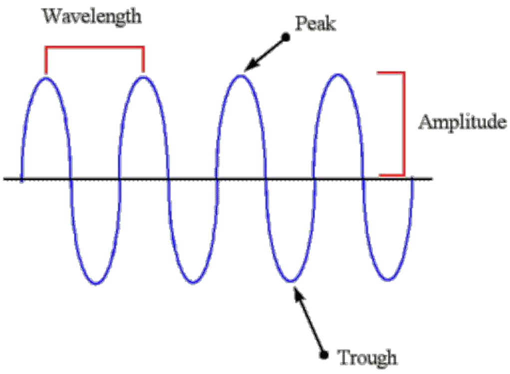
7.6 Electron Configuration

7.7 The Building-up Principle

7.1 From Classical Physics To Quantum Theory

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

Speed of the wave (u) = $\lambda\nu$

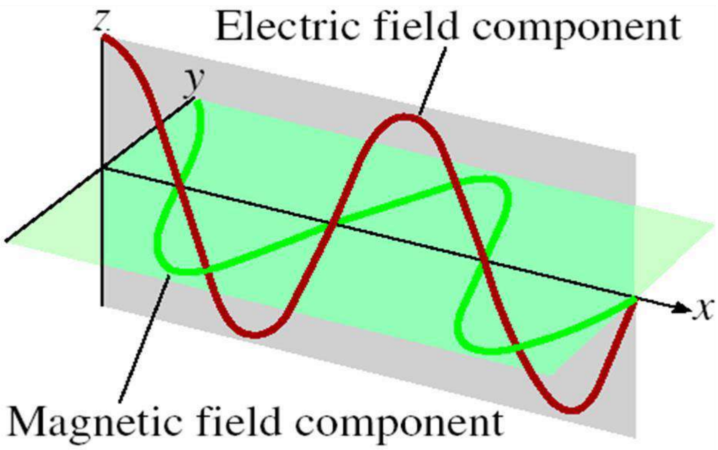
Maxwell's Electromagnetic Radiation Theory

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

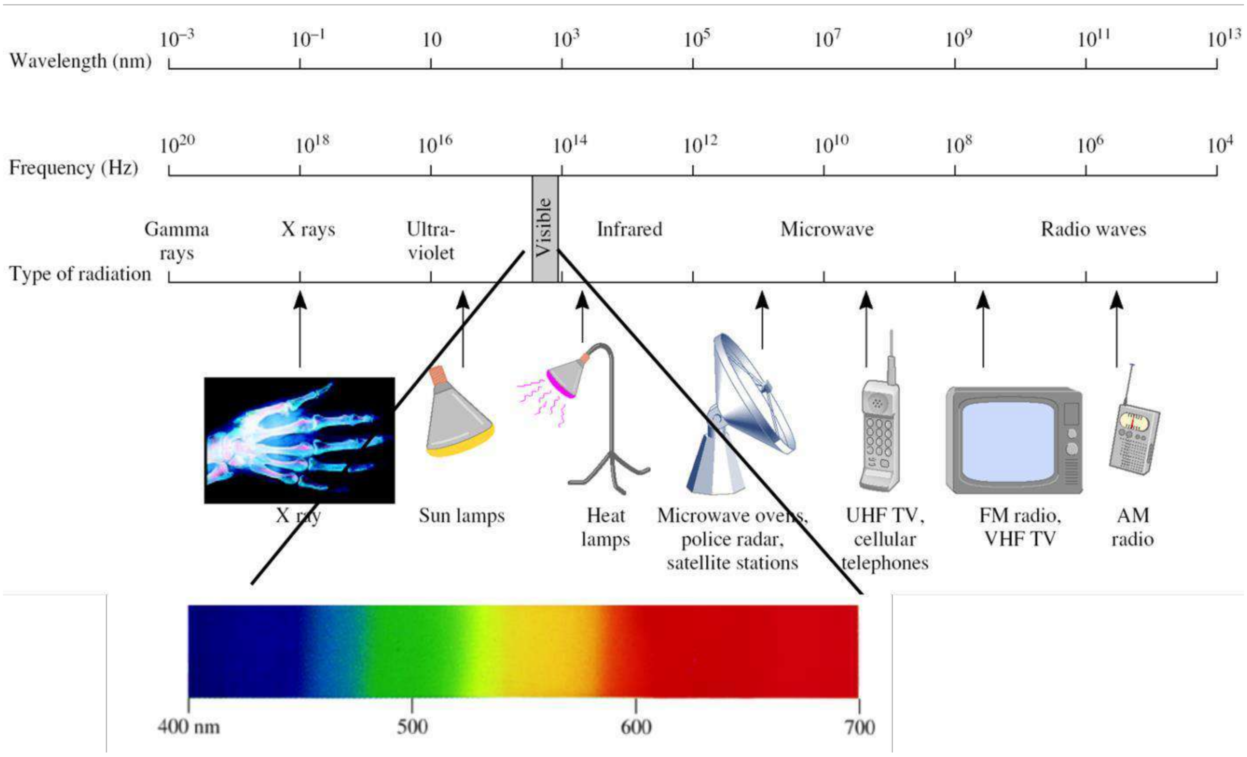
Electromagnetic radiation is the emission and transmission of energy in the form of electromagnetic waves.

Speed of light (c) = $\lambda\nu$

$= 3.00 \times 10^8$ m/s



Types of electromagnetic radiation



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

$$\lambda \nu = c$$

$$\lambda = c/\nu$$

$$\lambda = 3.00 \times 10^{8}\ \text{m/s} / 6.0 \times 10^{4}\ \text{Hz}$$

$$\lambda = 3.00 \times 10^{8}\ \text{m/s} / 6.0 \times 10^{4}\ \text{/s}$$

$$\lambda = 5.0 \times 10^{3}\ \text{m}$$

$$\lambda = 5.0 \times 10^{12}\ \text{nm}$$

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)

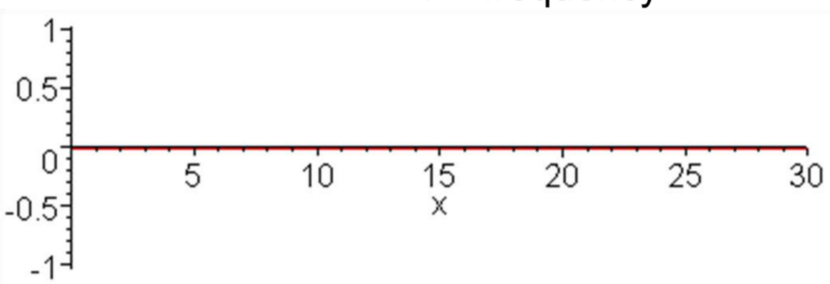
Quantum = the smallest quantity of energy that can be emitted/absorbed in the form of electromagnetic radiation.

Quantum energy, $E = h\nu$

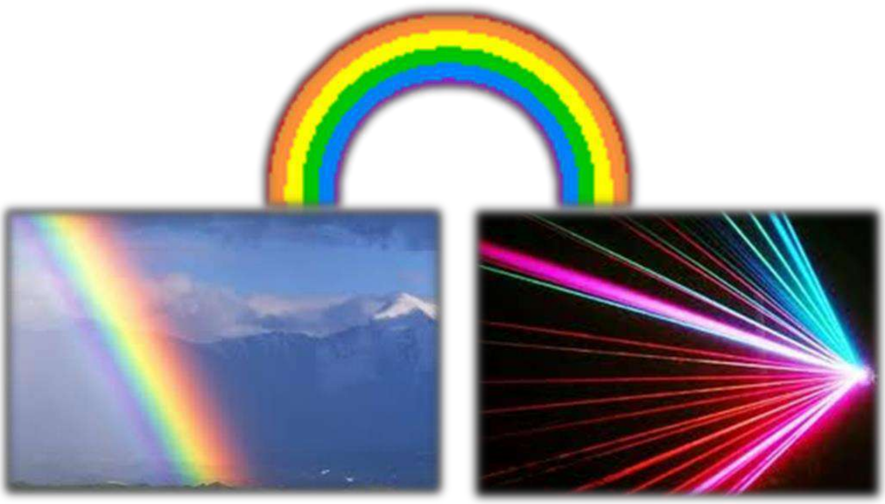
h = Planck's constant

= 6.63×10^{-34} Js

v = frequency

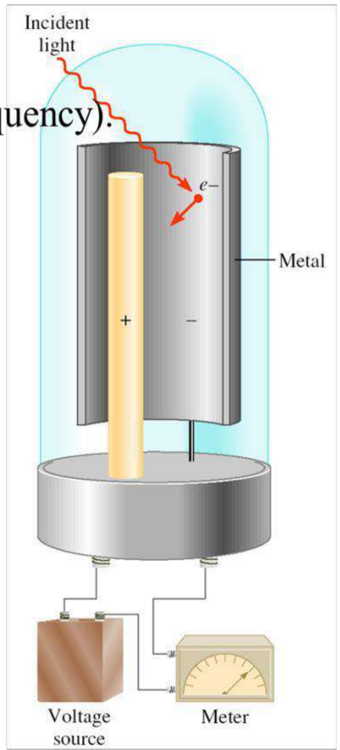


7.2 The Photoelectric Effect

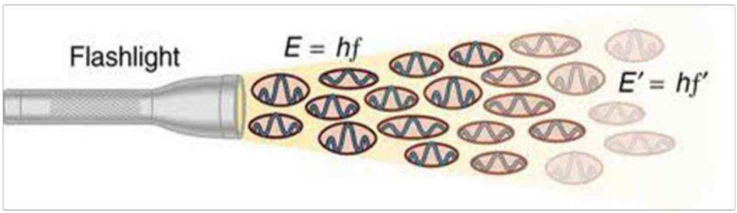


Einstein's light theory

Photoelectric Effect = electrons are ejected from the surface of certain metals exposed to light of at least a minimum frequency(threshold frequency).



Photon = particle of light

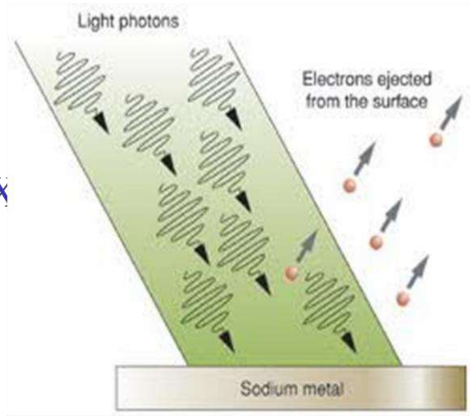


Photon energy, E = $h\nu$

Energy α frequency

Light has both **wave** and **particle**-like properties

When sodium is bombarded with high-energy 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.



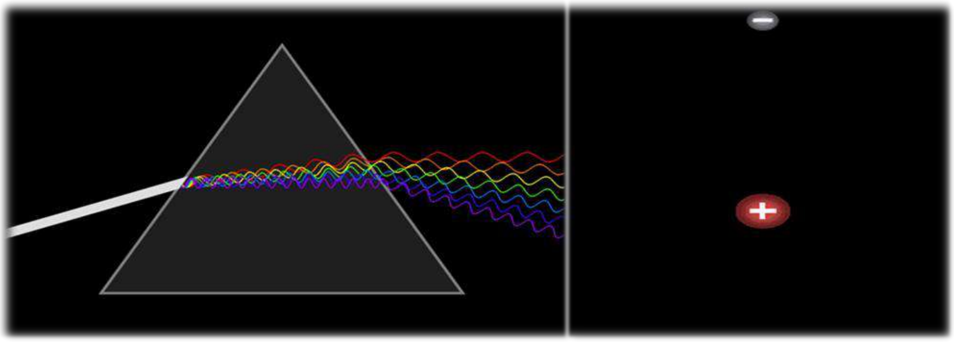
$$E = h\nu$$

$$E = h \times c / \lambda$$

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

$$E = 1.29 \times 10^{-15}\ \text{J}$$

7.3 Bohr's Theory Of The Hydrogen Atom

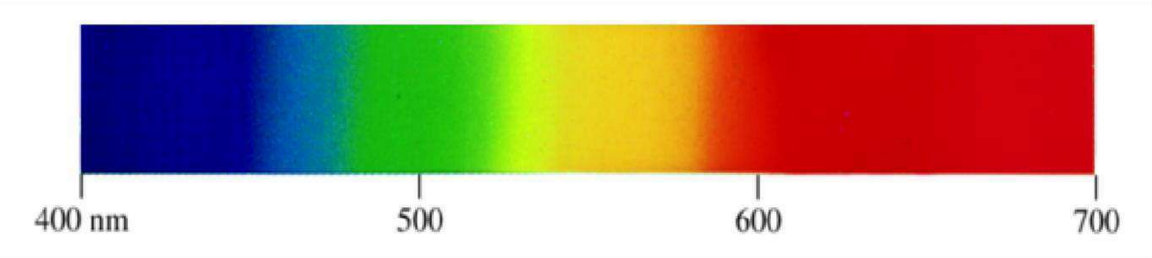


Emission spectra

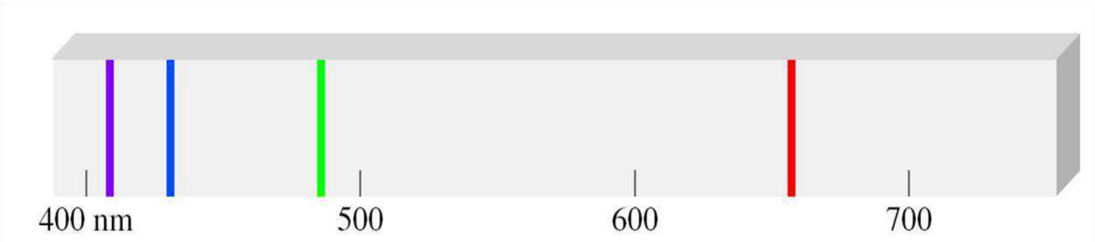
•Continuous/line spectra of radiation emitted by substances

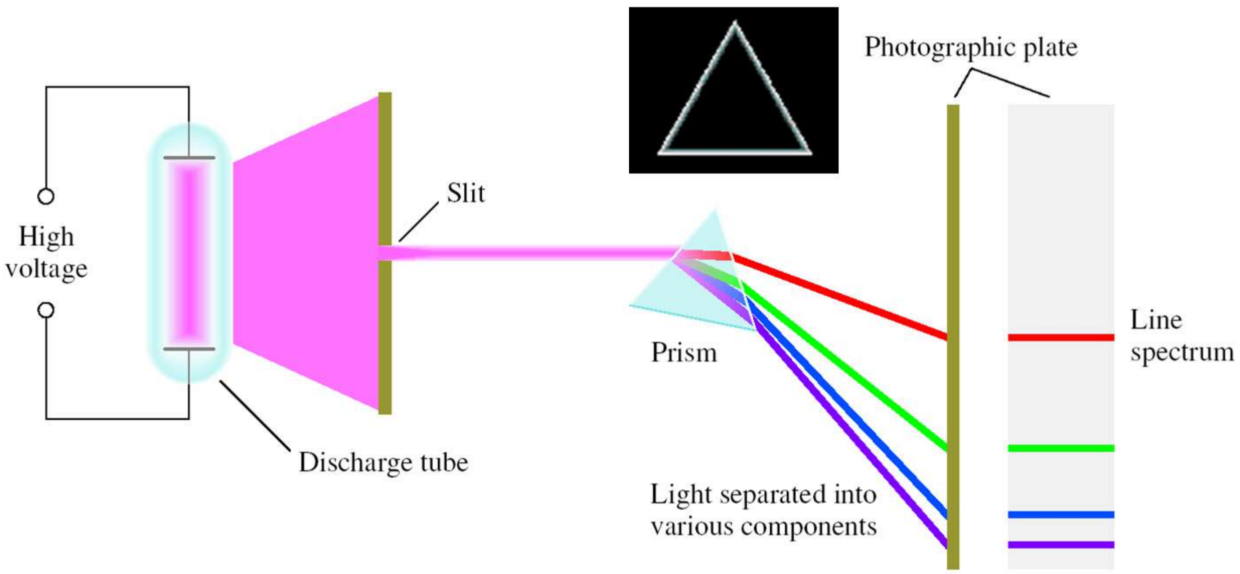
•Every element has a unique emission spectrum.

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

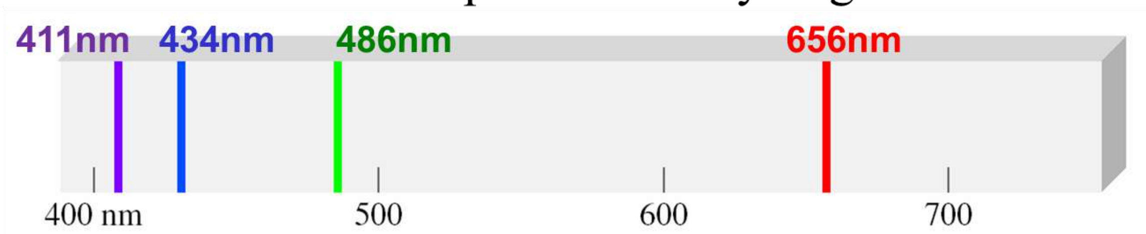


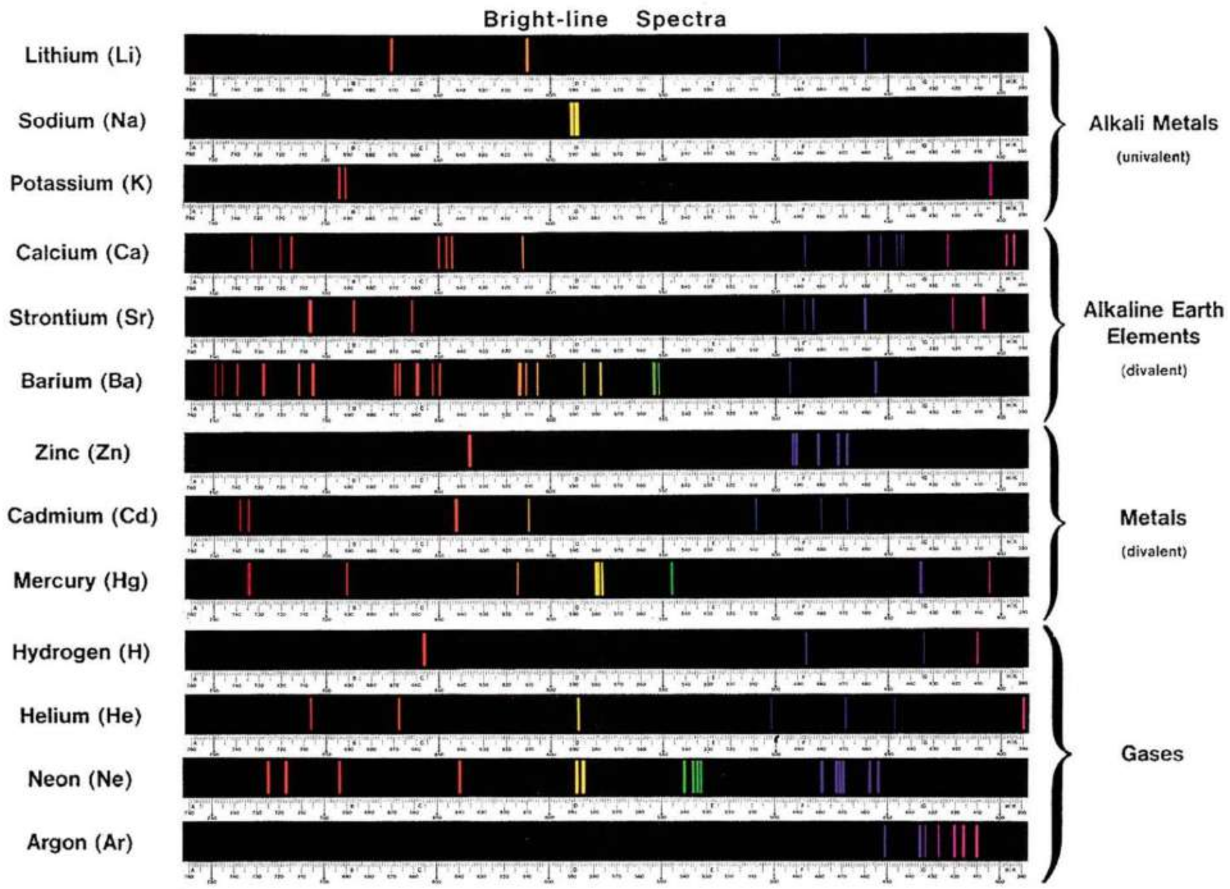
line spectra = light emission only at specific wavelengths,
eg H atom





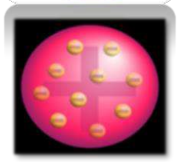
Line Emission Spectrum of Hydrogen Atoms

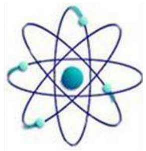




Bohr's Theory of Atom

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



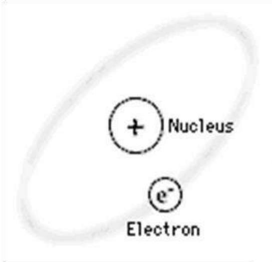


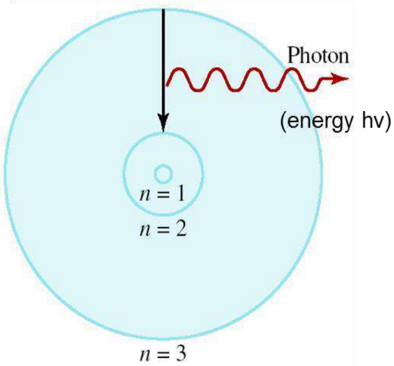
1. **e^- have specific (quantized) energy level**
2. **light is emitted as e^- moves from higher energy orbit to a lower-energy orbit**

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

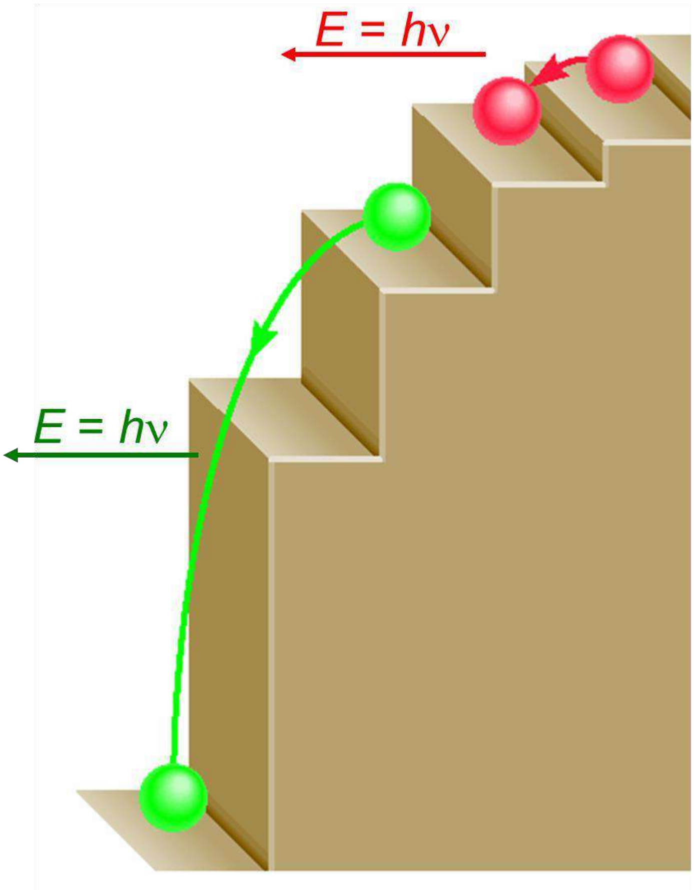
R_H = Rydberg constant
= 2.18×10^{-18} J

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,…)



$$E_{photon} = \Delta E = E_f - E_i$$

$$E_f = -R_H\left(\frac{1}{n_f^2}\right)$$

$$E_i = -R_H\left(\frac{1}{n_i^2}\right)$$

$$\Delta E = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$\Delta E = h\nu = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$n_i > n_f$
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.

$$E_{photon} = \Delta E = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

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

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

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

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

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

$$\lambda = 1280\ nm$$

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?

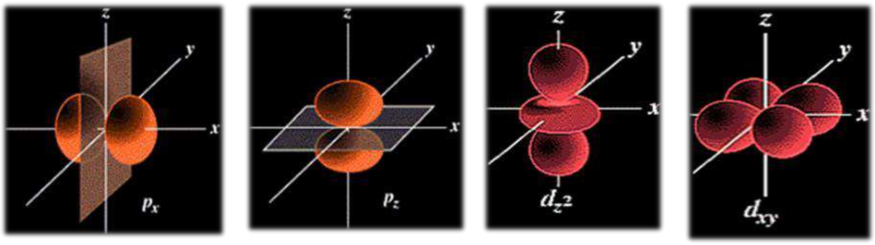
$\lambda = h/mu$

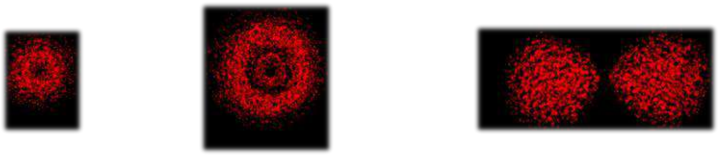
$\lambda = 6.63 \times 10^{-34} / (2.5 \times 10^{-3} \times 15.6)$

$\lambda = 1.7 \times 10^{-32}$ m

$\lambda = 1.7 \times 10^{-23}$ nm

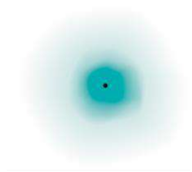
7.5 Quantum Numbers



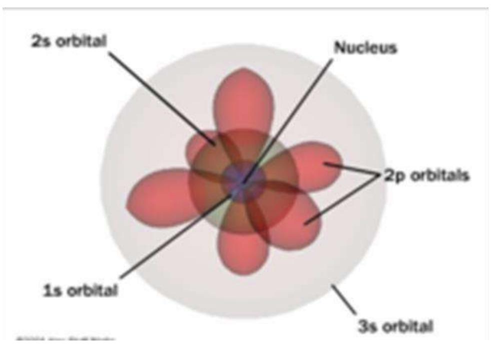


Quantum numbers

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.

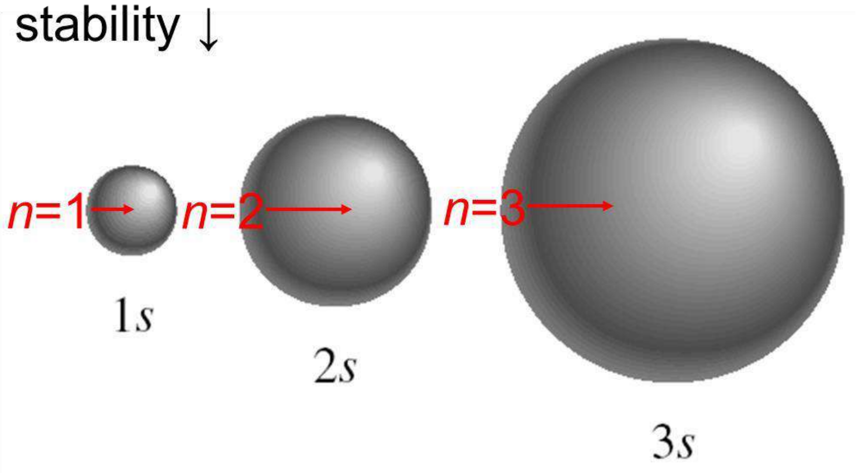


1)Principal quantum number (n)
2)Angular momentum quantum number (l)
3)Magnetic quantum number (m_l)
4)Spin quantum number (m_s)



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 ↓



Angular momentum quantum number (l)

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

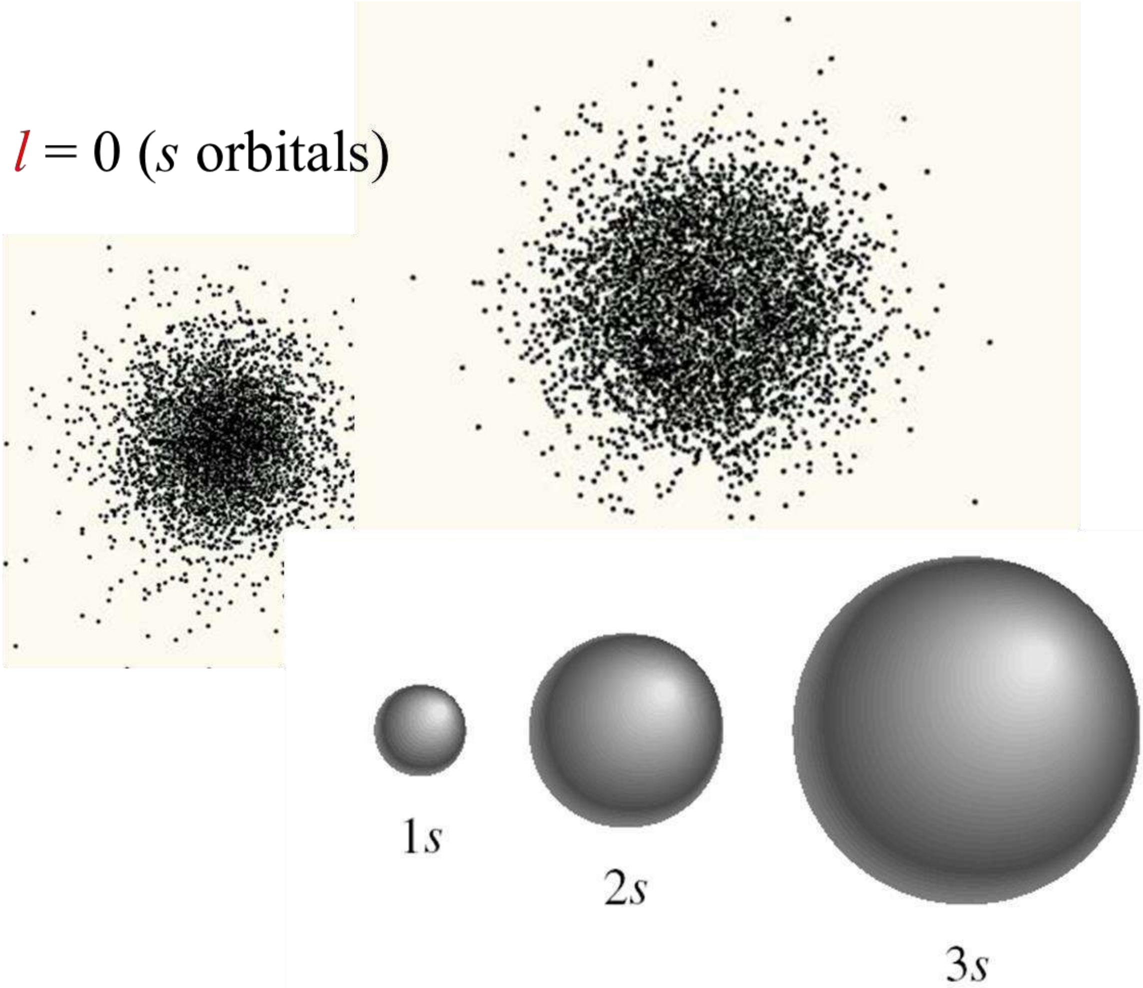
possible values = 0 1 2 3 4 5………… *n*-1

letter designation = *s p d f g h*………….

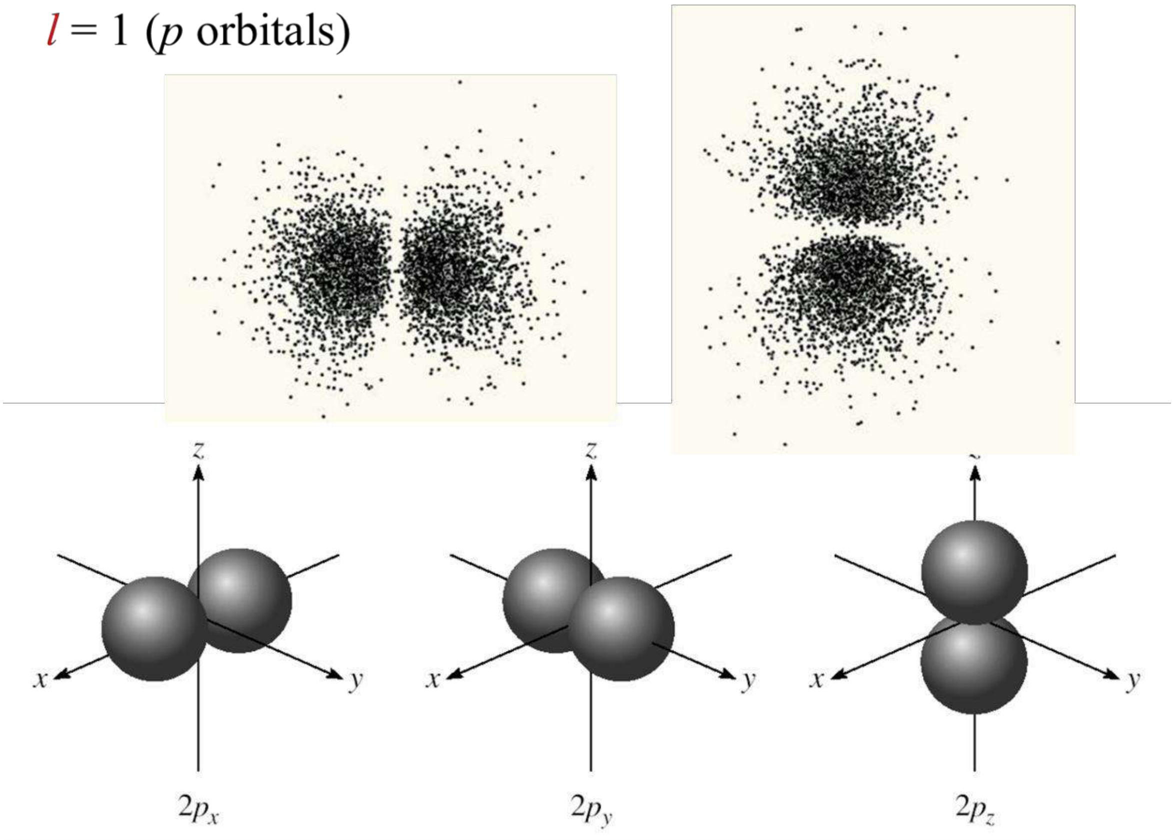
values of *n*	values of *ℓ*	orbitals
1	0	1*s*
2	0, 1	2*s*, 2*p*
3	0, 1, 2	3*s*, 3*p*, 3*d*

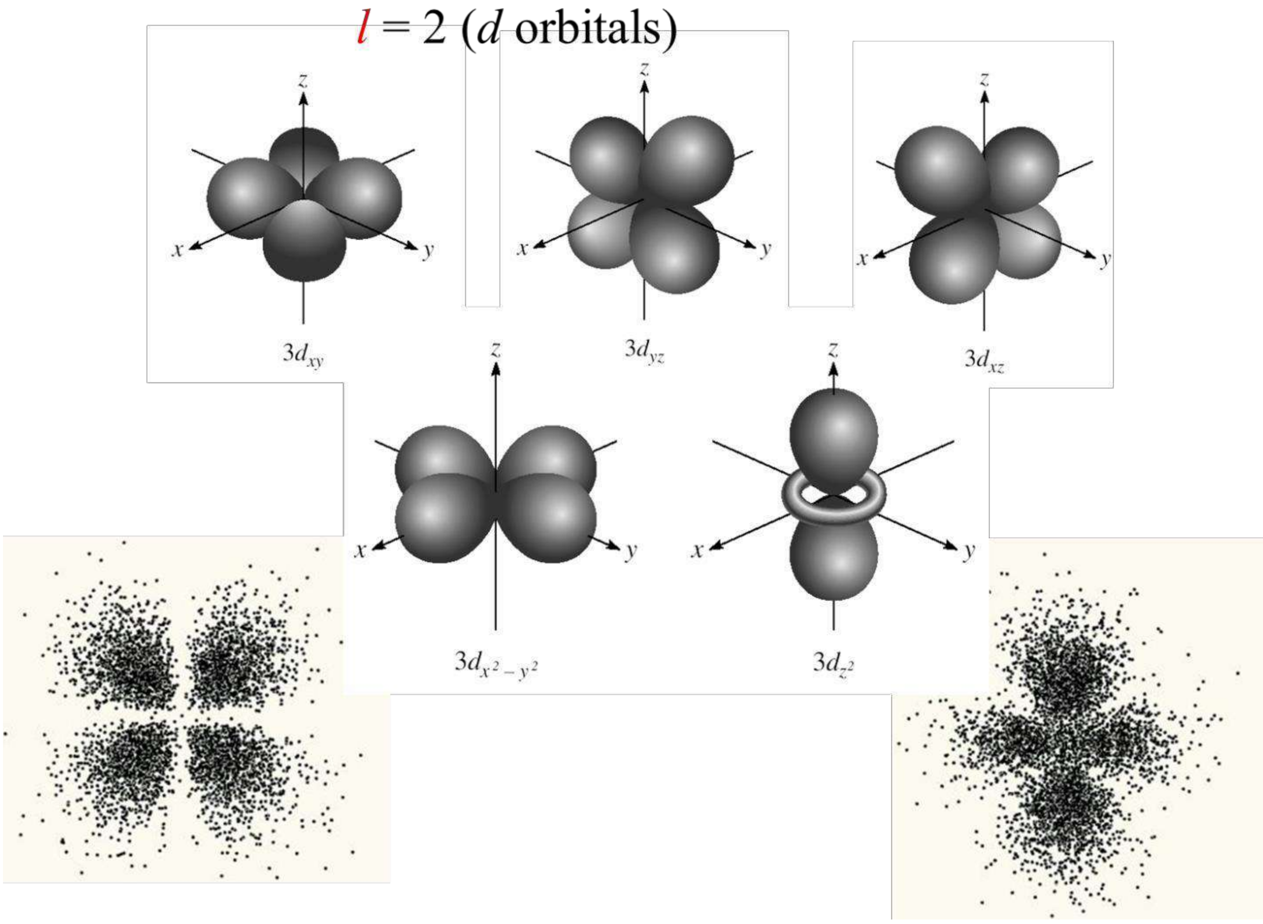
shells → subshells → orbitals

$l = 0$ (s orbitals)



$l = 1$ (p orbitals)





Magnetic quantum number (m_l)

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

within subshell ℓ = 2, there are 5 orbitals corresponding to the 5 possible values of m_ℓ (- 2, -1, 0, +1, +2)

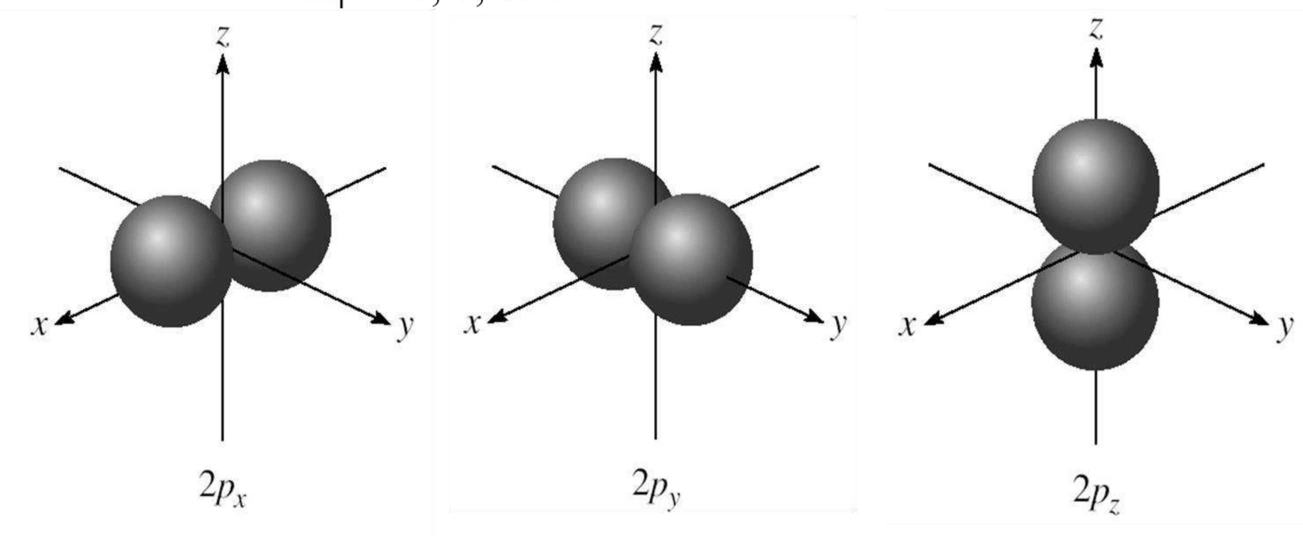
d orbitals come in sets of 5 (- 2, -1, 0, +1, +2)

p orbitals in sets of 3 (-1, 0, +1)

s orbitals in sets of 1 (0)

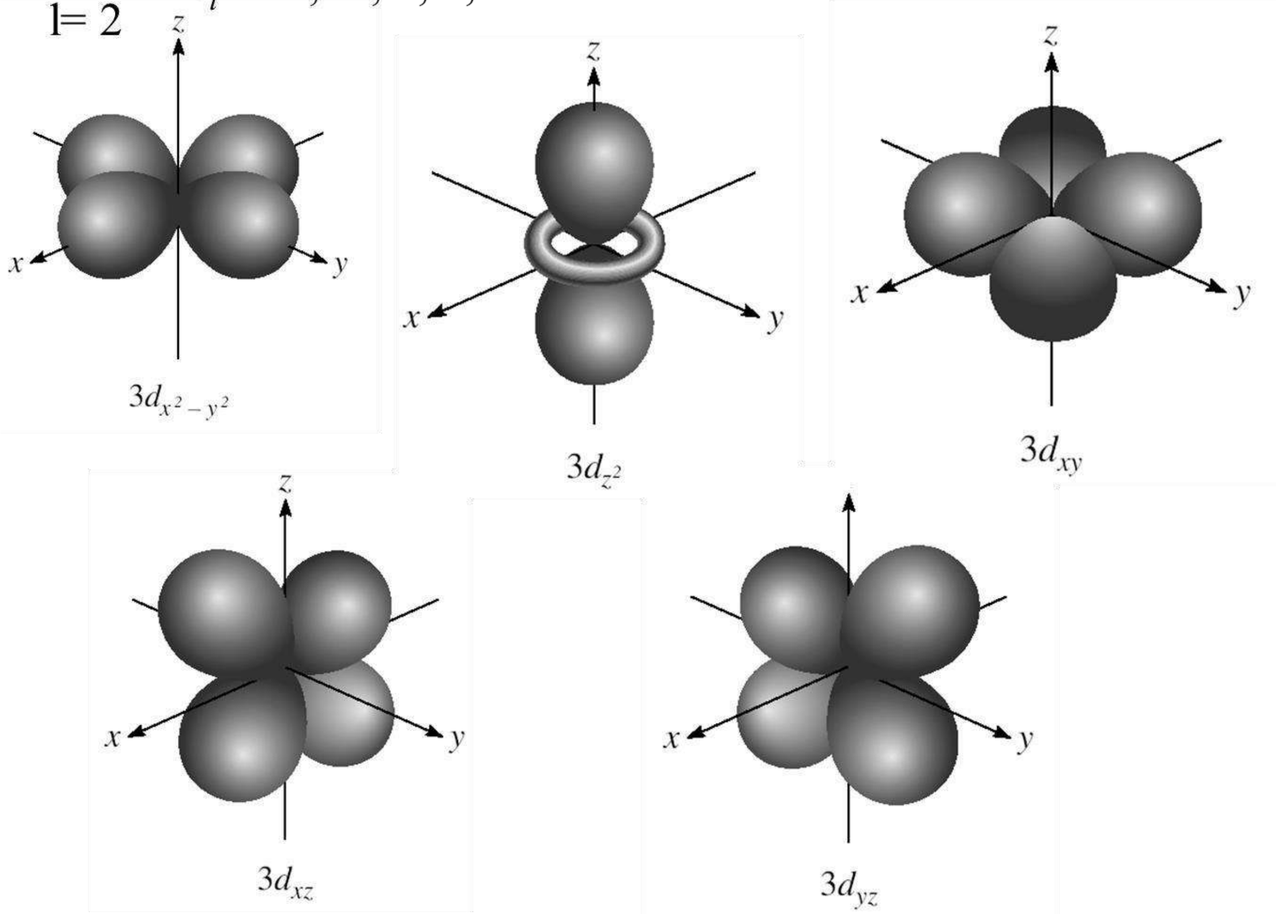
n= 2
l=1
m_l = -1, 0, **or** 1

3 orientations is space



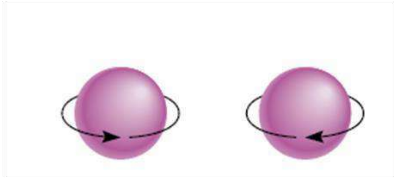
n= 3
l= 2

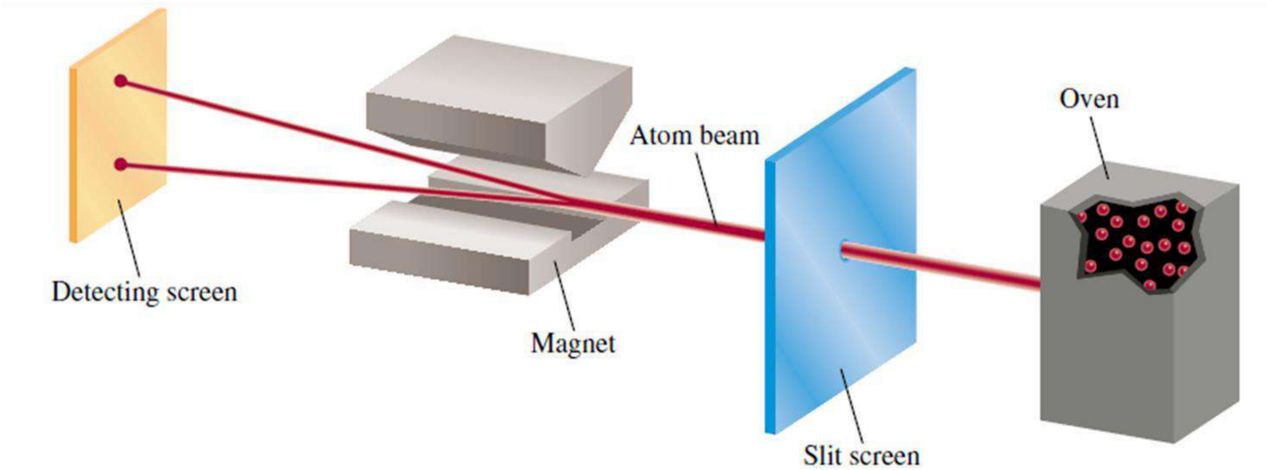
m_l = -2, -1, 0, 1, **or** 2 5 orientations is space

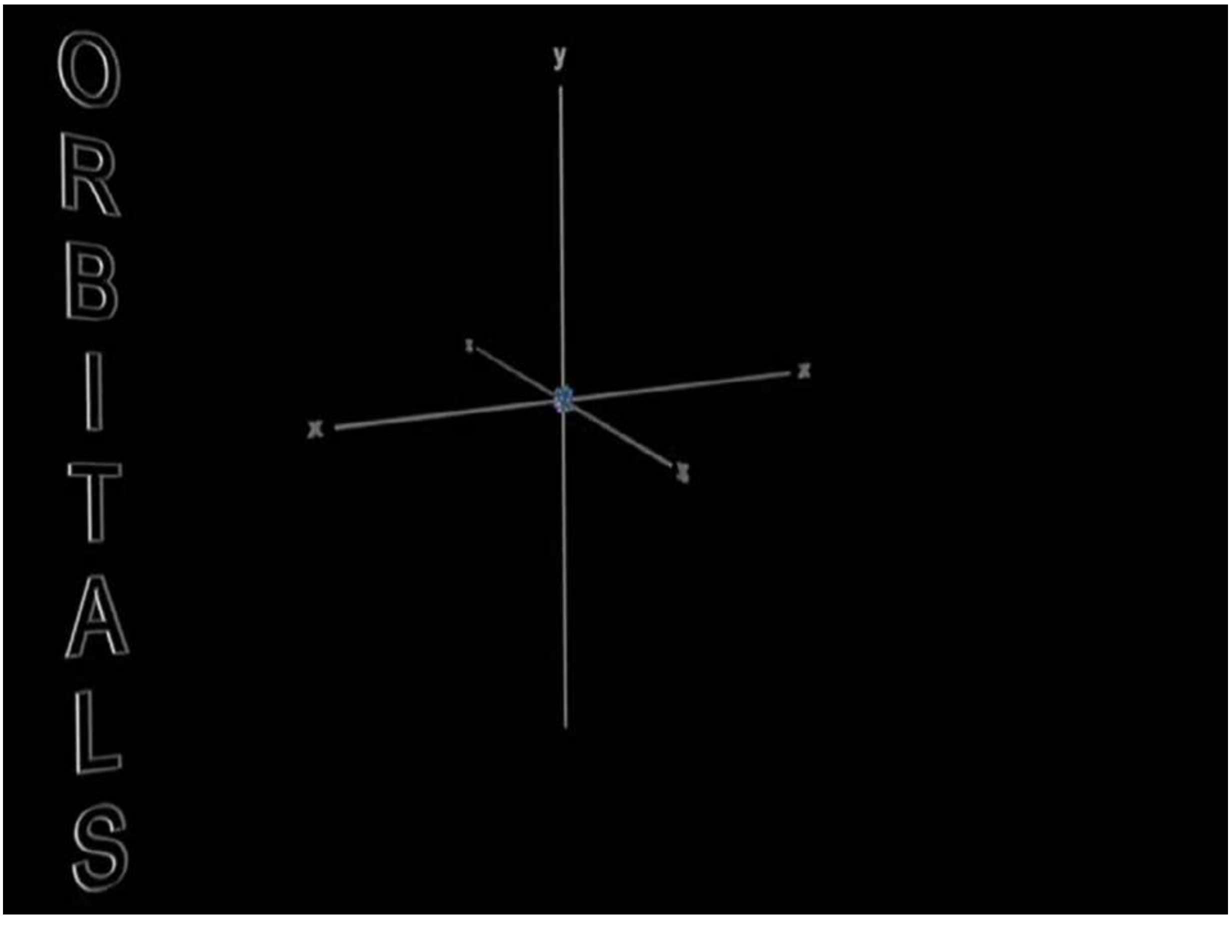


Electron spin quantum number (m_s)

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





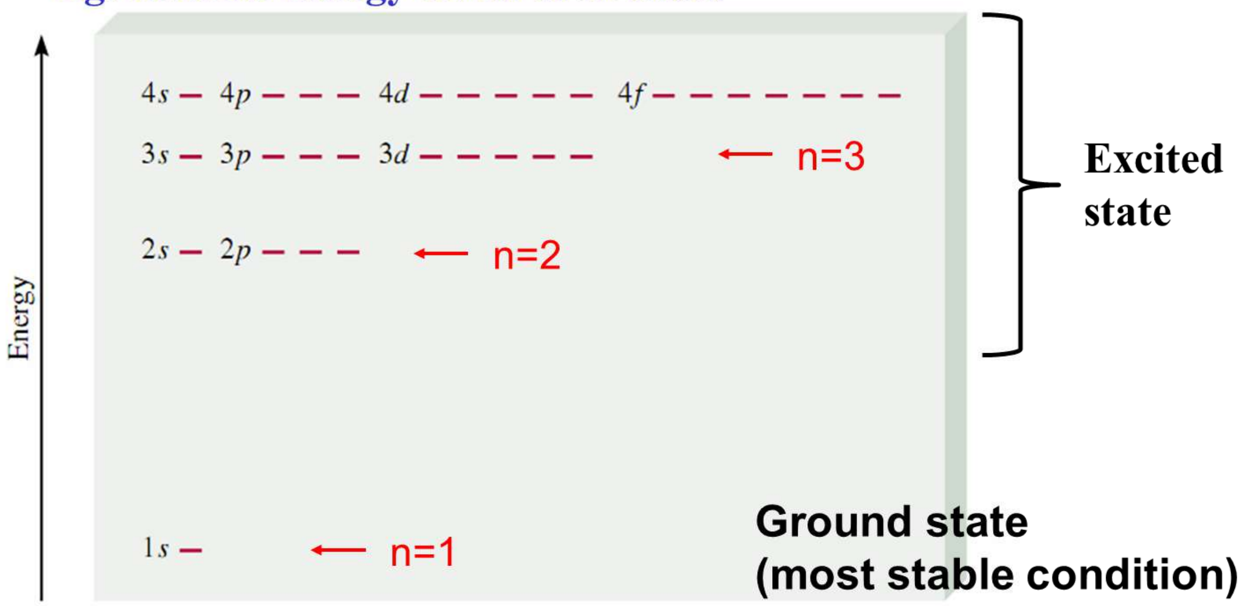


Atomic orbital

n	ℓ	m_ℓ	subshell	# orbitals
1	0	0	1*s*	1
2	0	0	2*s*	1
	1	-1. 0, +1	2*p*	3
3	0	0	3*s*	1
	1	-1, 0, +1	3*p*	3
	2	-2, -1, 0, +1, +2	3*d*	5
4	0	0	4*s*	1
	1	-1, 0, +1	4*p*	3
	2	-2, -1, 0, +1, +2	4*d*	5
	3	-3, -2, -1, 0, +1, +2, +3	4*f*	7

Energy of Orbitals in a single e- atom

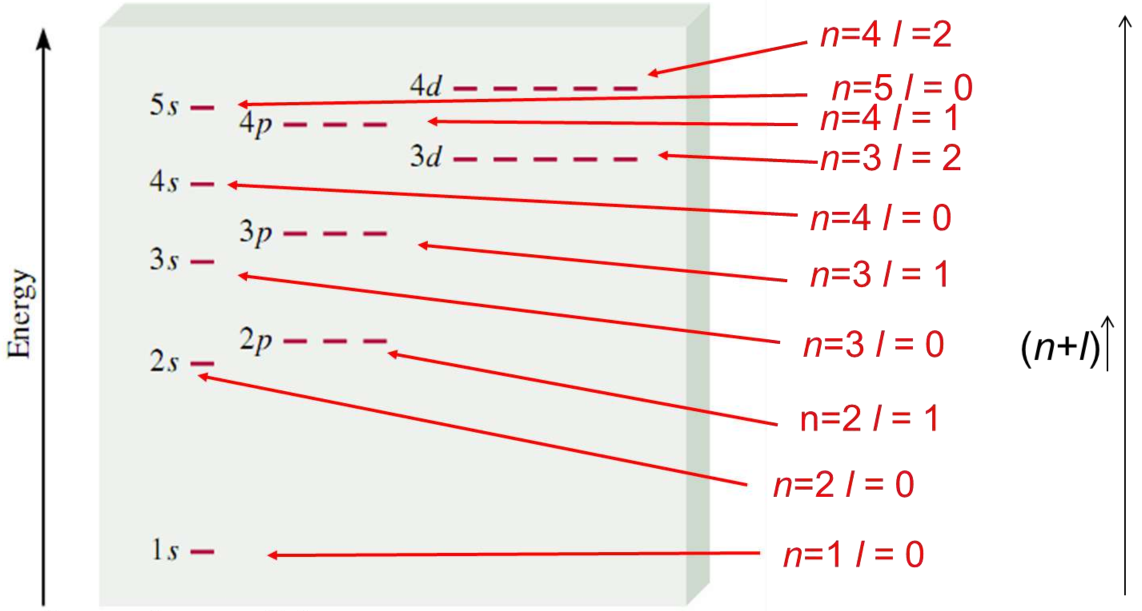
Eg. orbitals energy levels in H atom



→ Energy only depends on principal quantum number ***n***

Energy of orbitals in a multi-electron atom (atom containing two or more e-)

Eg. orbitals energy levels in many-electron atom



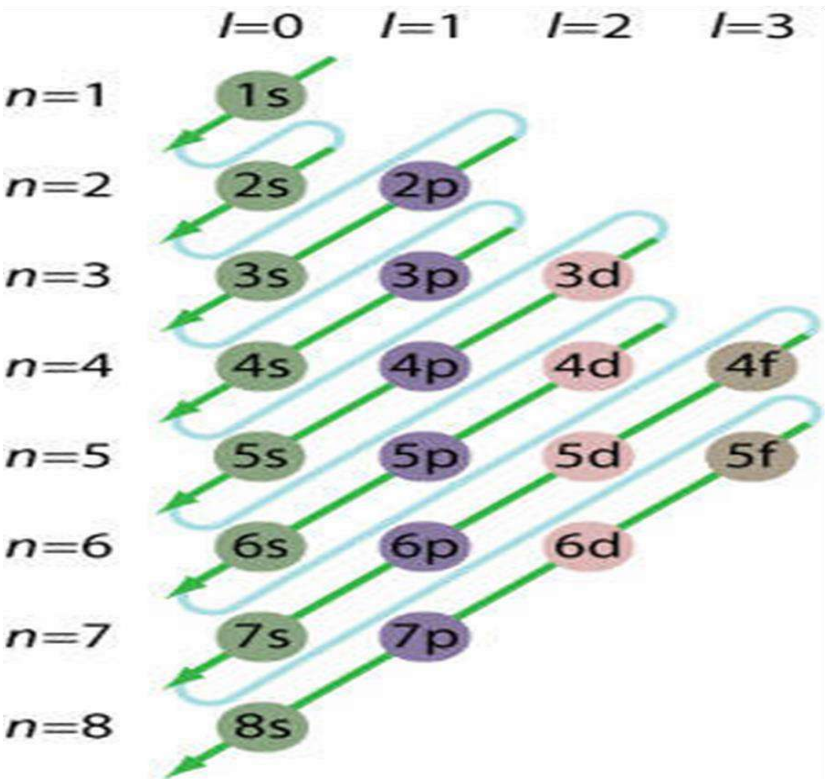
→ depend on n & l

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

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

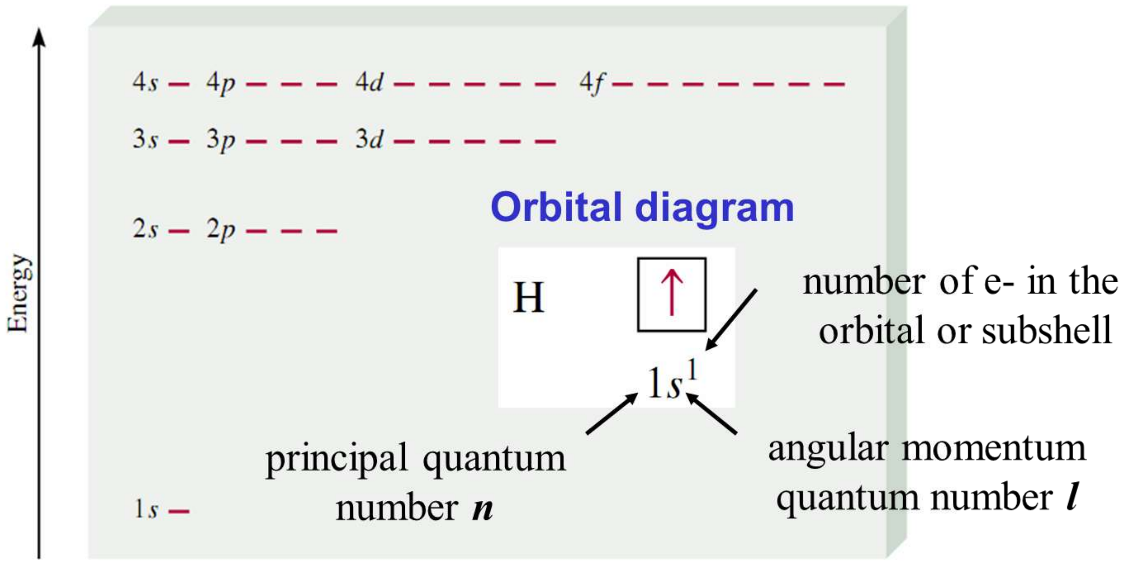
Order of orbitals (filling) in multi-electron atom

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



7.6 Electron Configuration

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



Quantum numbers: (n, l, m_l, m_s)

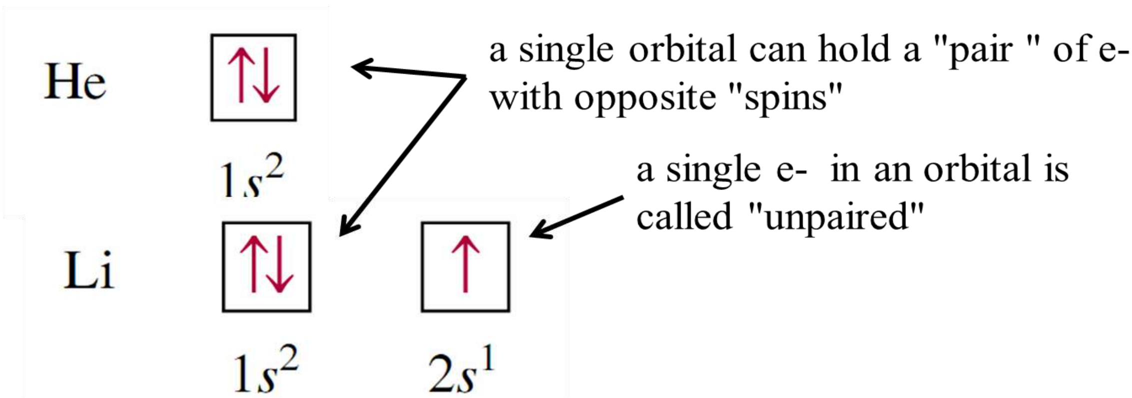
Each electron's quantum numbers are unique and cannot be shared by another electron in that atom.

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

→ ∴ maximum of 2 electrons per orbital

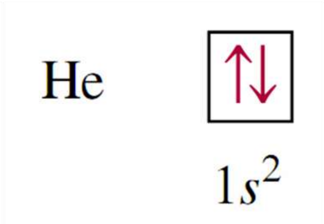
atomic number (Z) = # protons = # electrons (in neutral atom)



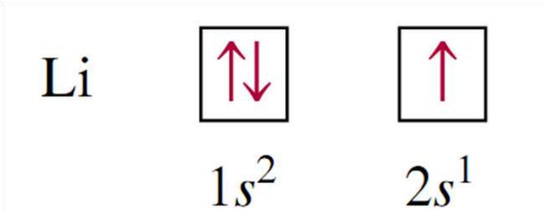
Paramagnetism and Diamagnetism

• atoms with 1 or more *unpaired electrons are* ***paramagnetic*****,**
(attracted by a magnetic)

• atoms with all spins *paired are* ***diamagnetic***
(repelled by magnet)



→ ***diamagnetic***

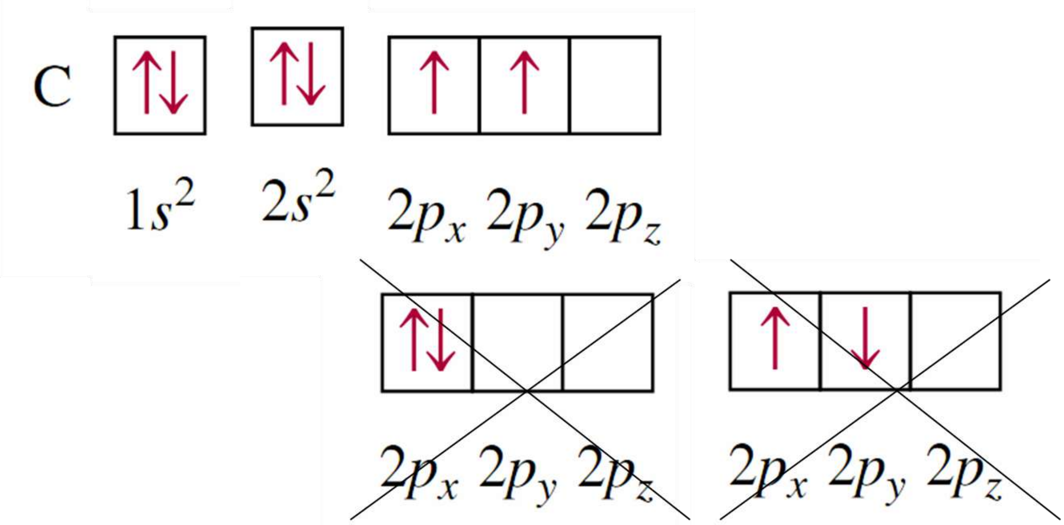


→ ***paramagnetic***

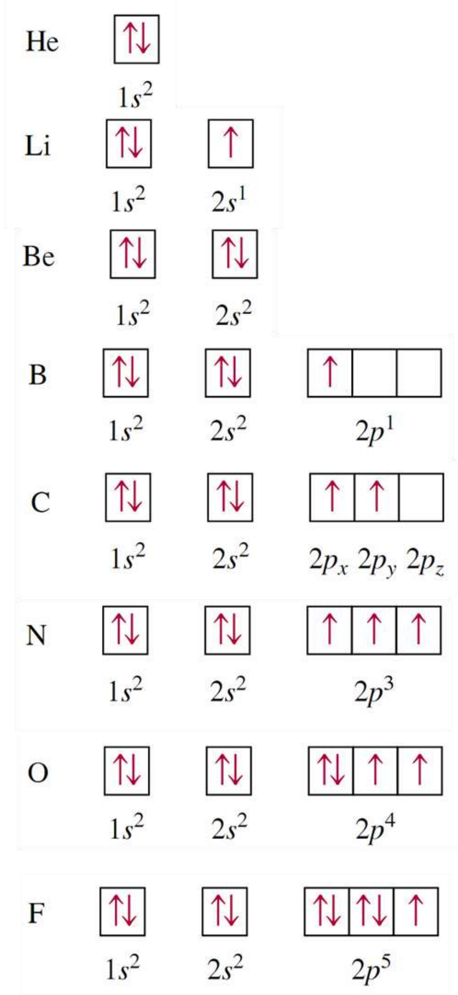
Hund's Rule

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

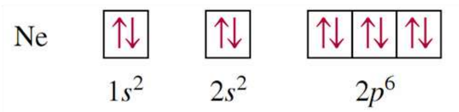
e- configuration of C (Z=6)



#	Atom	Electron Configuration
1	H	$1s^1$
2	He	$1s^2$
3	Li	$1s^2\ 2s^1$
4	Be	$1s^2\ 2s^2$
5	B	$1s^2\ 2s^2\ 2p^1$
6	C	$1s^2\ 2s^2\ 2p^2$
7	N	$1s^2\ 2s^2\ 2p^3$
8	O	$1s^2\ 2s^2\ 2p^4$
9	F	$1s^2\ 2s^2\ 2p^5$
10	Ne	$1s^2\ 2s^2\ 2p^6$



[Ne] ←



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

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

n = 3	ℓ =	0	1	2
	subshell	3s	3p	3d
	# 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?

n=2

↓

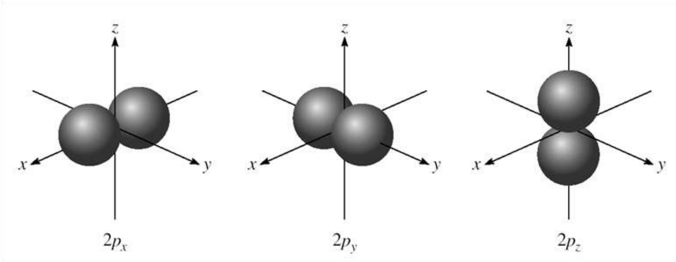
2*p*

↑

l = 1

If l = 1, then m_l = -1, 0, or +1

3 orbitals



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

n=3

↓

3*d*

↑

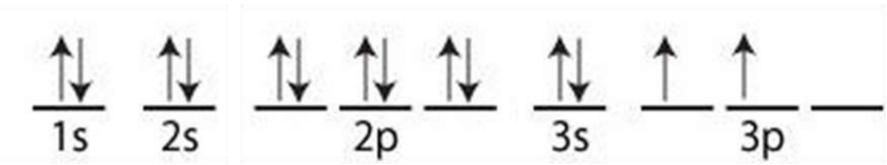
l = 2

If l = 2, then m_l = -2, -1, 0, +1, or +2

5 orbitals which can hold a total of 10 e^-

Determine the electron configuration of silicon

Silicon has 14 protons and 14 electrons



The electron configuration of silicon is $1s^2 2s^2 2p^6 3s^2 3p^2$

7.7 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] $=1s^2 2s^2 2p^6$

[Ar] $=1s^2 2s^2 2p^6 3s^2 3p^6$

e- configuration of Na

$\rightarrow 1s^2 2s^2 2p^6 3s^1$

or

$\rightarrow$ [Ne] $3s^1$

- 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] $4s^1 3d^5$ instead of [Ar] $4s^2 3d^4$
Cu (Z=29), the e- configuration is [Ar] $4s^1 3d^{10}$ instead of [Ar]$4s^2 3d^9$

Because of greater stability associated with half-filled ($3d^5$)and completely filled ($3d^{10}$)subshells

What is the electron configuration of Mg?

Mg 12 electrons

1s < 2s < 2p < 3s < 3p < 4s

$1s^2 2s^2 2p^6 3s^2$ 2 + 2 + 6 + 2 = 12 electrons

Abbreviated as [Ne]$3s^2$ [Ne] $=1s^2 2s^2 2p^6$

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

Cl 17 electrons 1s < 2s < 2p < 3s < 3p < 4s

$1s^2 2s^2 2p^6 3s^2 3p^5$ 2 + 2 + 6 + 2 + 5 = 17 electrons

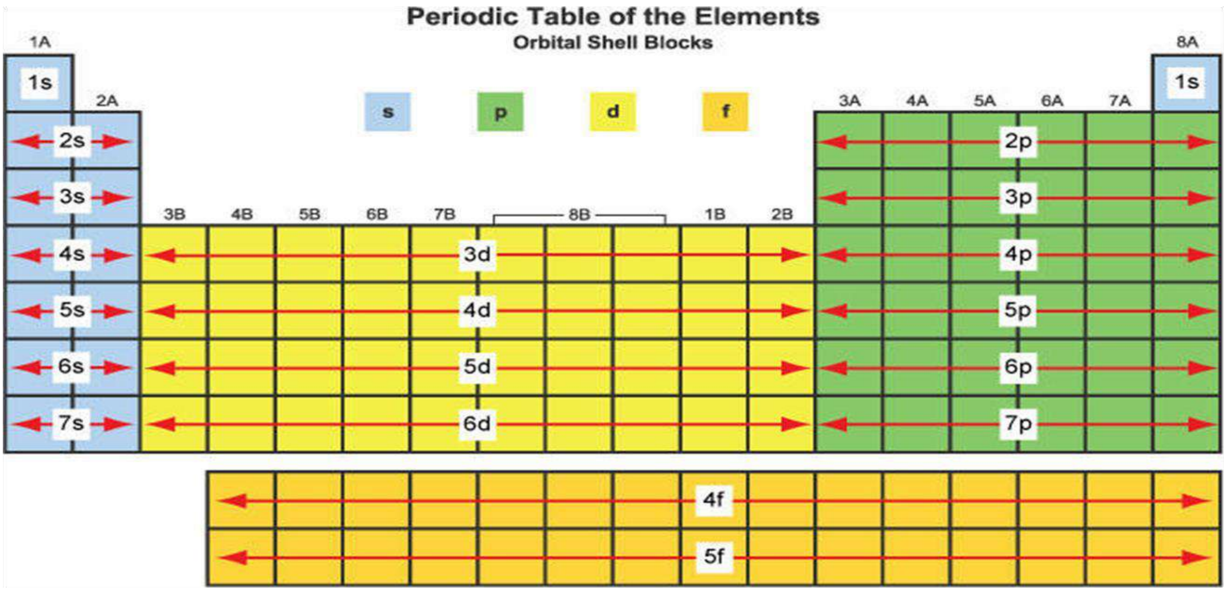
Last electron added to 3p orbital

$n = 3$ $l = 1$ $m_l = -1, 0, \text{ or } +1$ $m_s = ½ \text{ or } -½$

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

ATOMIC NUMBER	SYMBOL	ELECTRON CONFIGURATION	ATOMIC NUMBER	SYMBOL	ELECTRON CONFIGURATION	ATOMIC NUMBER	SYMBOL	ELECTRON CONFIGURATION
1	H	$1s^{1}$	37	Rb	[Kr]$5s^{1}$	73	Ta	[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	B	[He]$2s^{2}2p^{1}$	41	Nb	[Kr]$5s^{1}4d^{4}$	77	Ir	[Xe]$6s^{2}4f^{14}5d^{7}$
6	C	[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	O	[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	P	[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]$6s^{2}4f^{1}5d^{1}$	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]$6s^{2}4f^{7}$	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	Ha	[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]$7s^{2}5f^{14}6d^{7}$

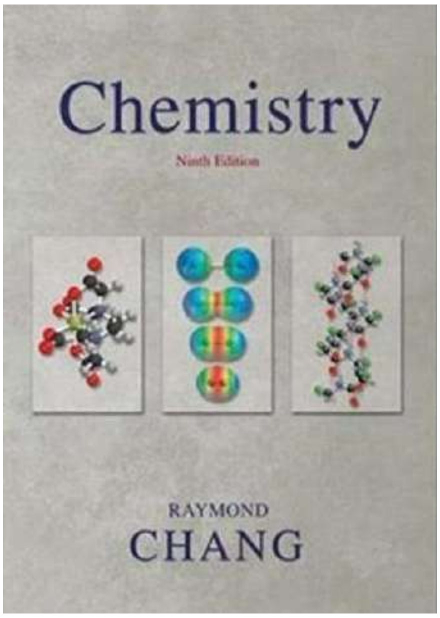
<u>Outermost subshell being filled with e-</u>



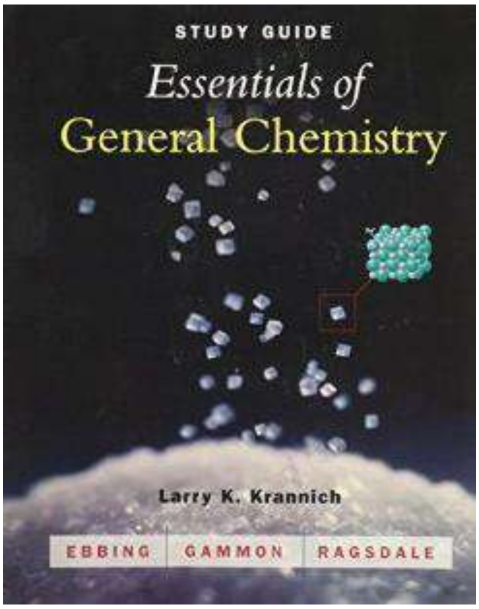
•***alkali metals*** *and* ***alkaline earth metals*** *fill the* ***s orbitals*** *last*
•***main group*** *elements fill the* ***p orbitals*** *last*
•***transition metals*** *fill the* ***d orbitals*** *last*
•***lanthanides (4f)*** *and* ***actinides (5f)*** *fill the* ***f orbitals*** *last*

Lecture References :

1. Raymond Chang ,General Chemistry, McGraw Hill 9th ed., 2007.

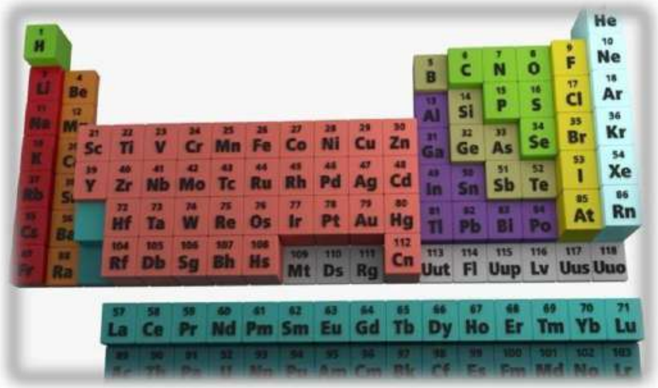


2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.



LECTURE 8

Periodic Relationships Among Elements



8.1 Periodic Classification of The Elements

8.2 Periodic Variation in Physical Properties

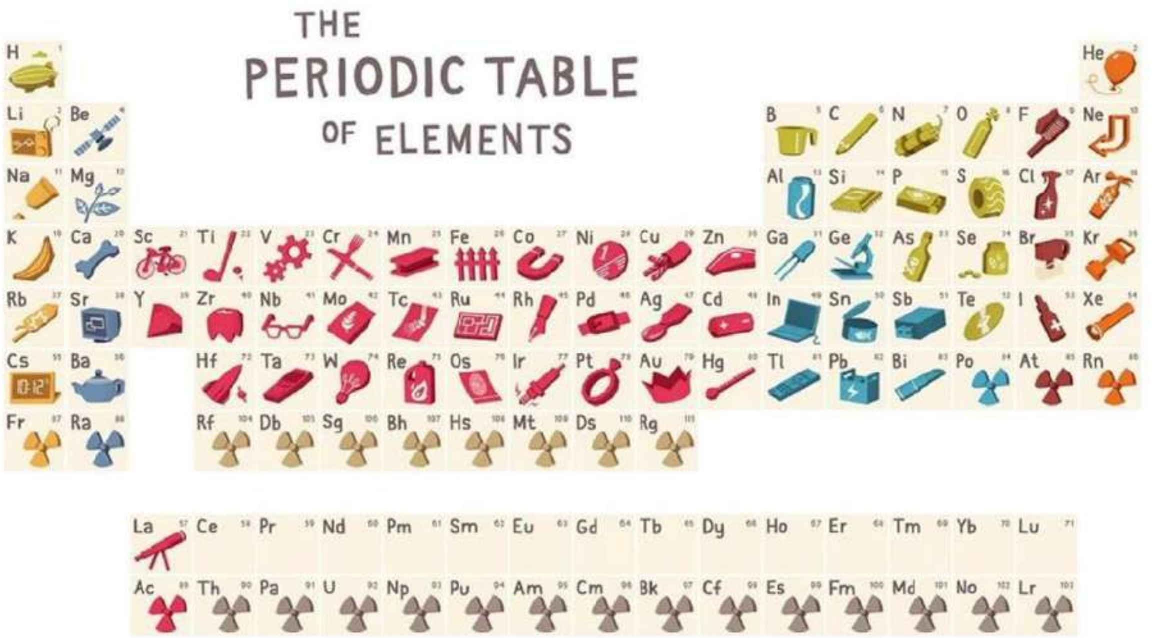
8.3 Ionization Energy

8.4 Electron Affinity

8.5 Variation in Chemical Properties of The Representative Elements

8.1 Periodic Classification of The Elements

- **Modern periodic table is based on Mendeleev's periodic table**
- **Elements are arranged according to increasing atomic number**



Categories of elements-correspond to which subshell is last filled

Representative elements (main group elements)

•Groups 1A to 7A

•Incompletely filled s or p subshell

Noble gases

•Group 8A

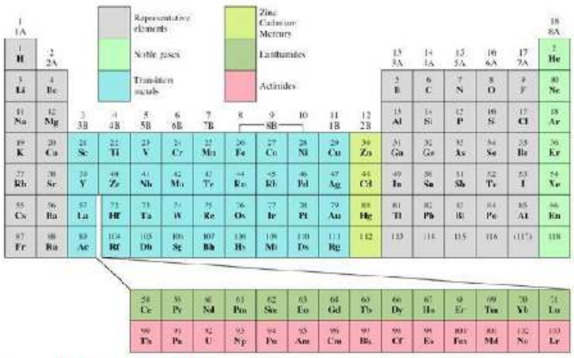
•Completely filled s or p subshell

Transition metals

•d-block elements

•Groups 1 B to 8 B

•Incompletely filled d subshells



Lanthanides (rare earth elements) and Actinides

•f- block elements

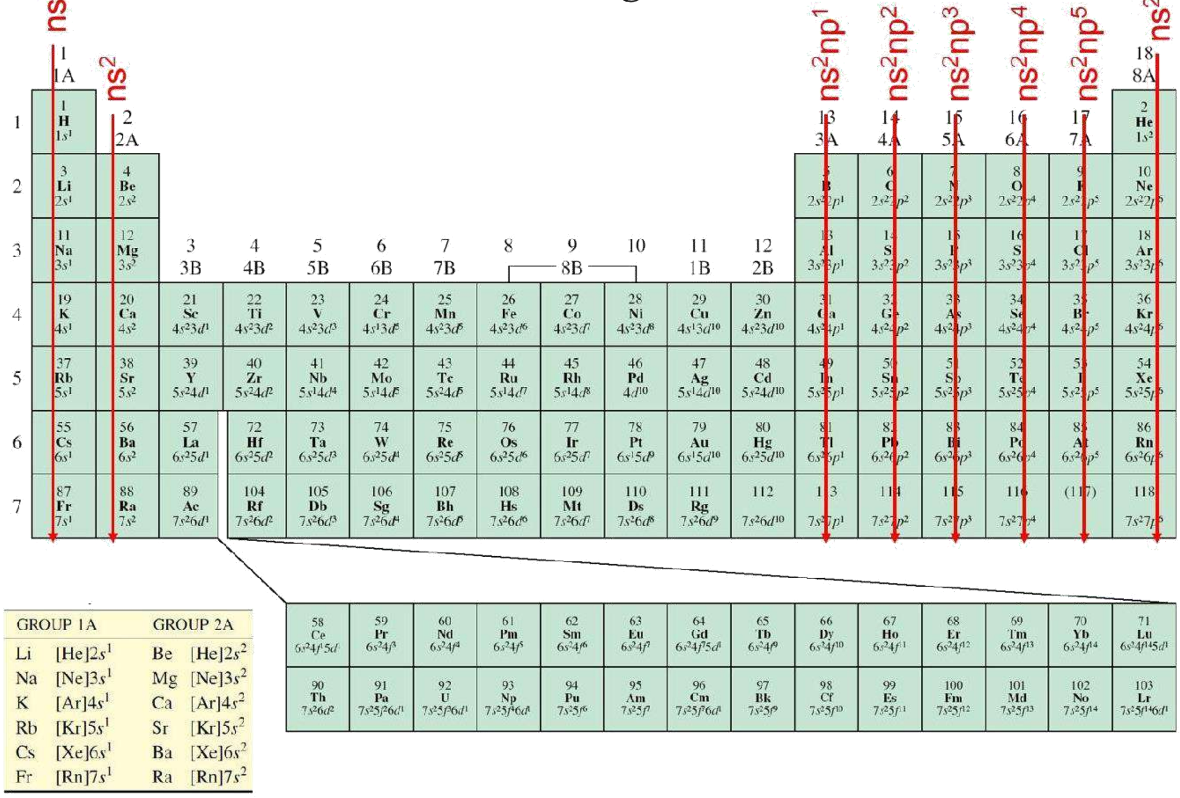
•Incompletely filled f subshells

Valence electrons

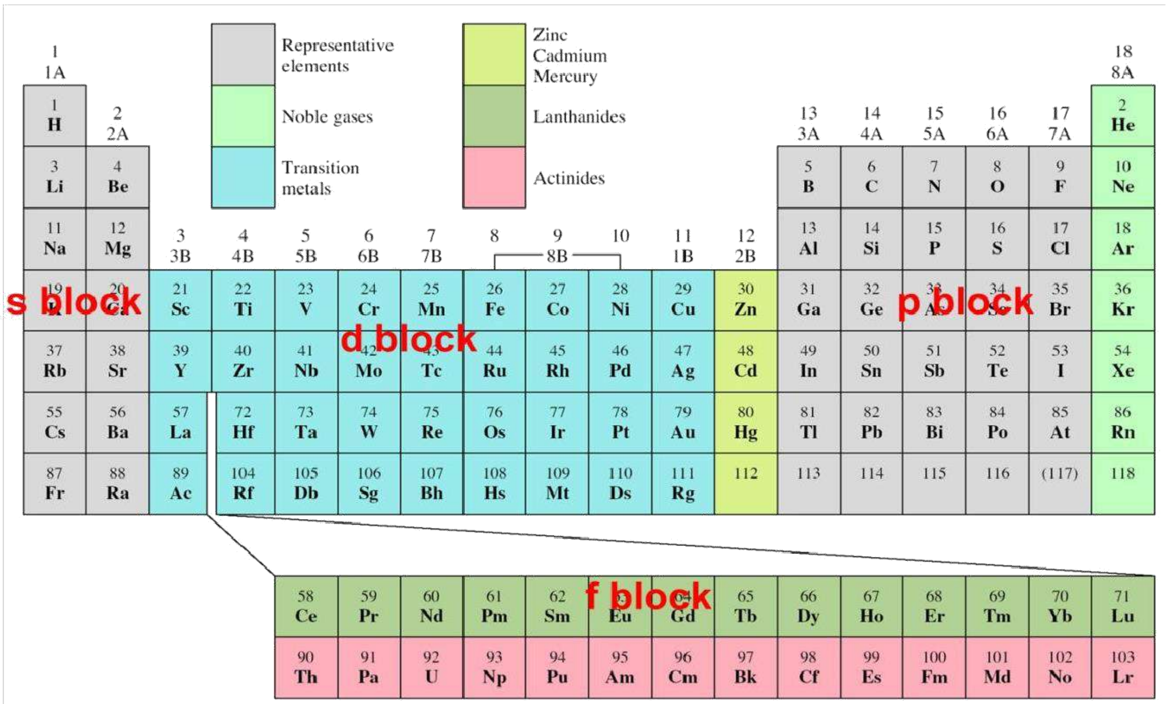
– the outer e- of an atom that involved in chemical bonding

– eg. Group 7A - all have ns^2np^5, Group 1A – all have ns^1 etc.

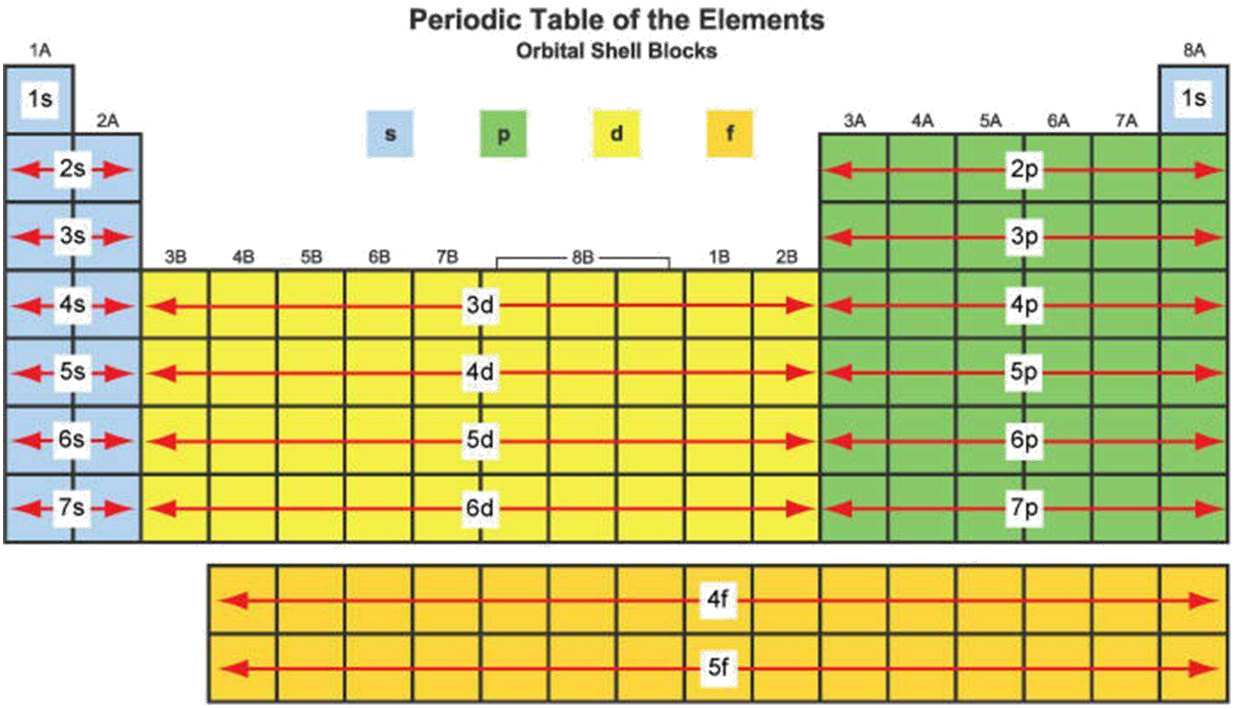
Ground State Electron Configurations of the Elements



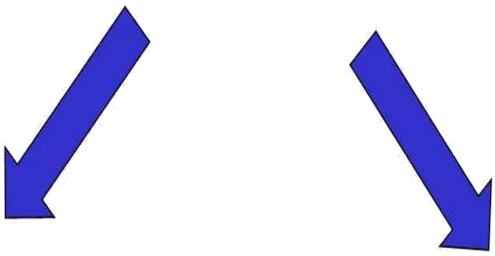
Classification of the Elements



Electron configuration and periodicity



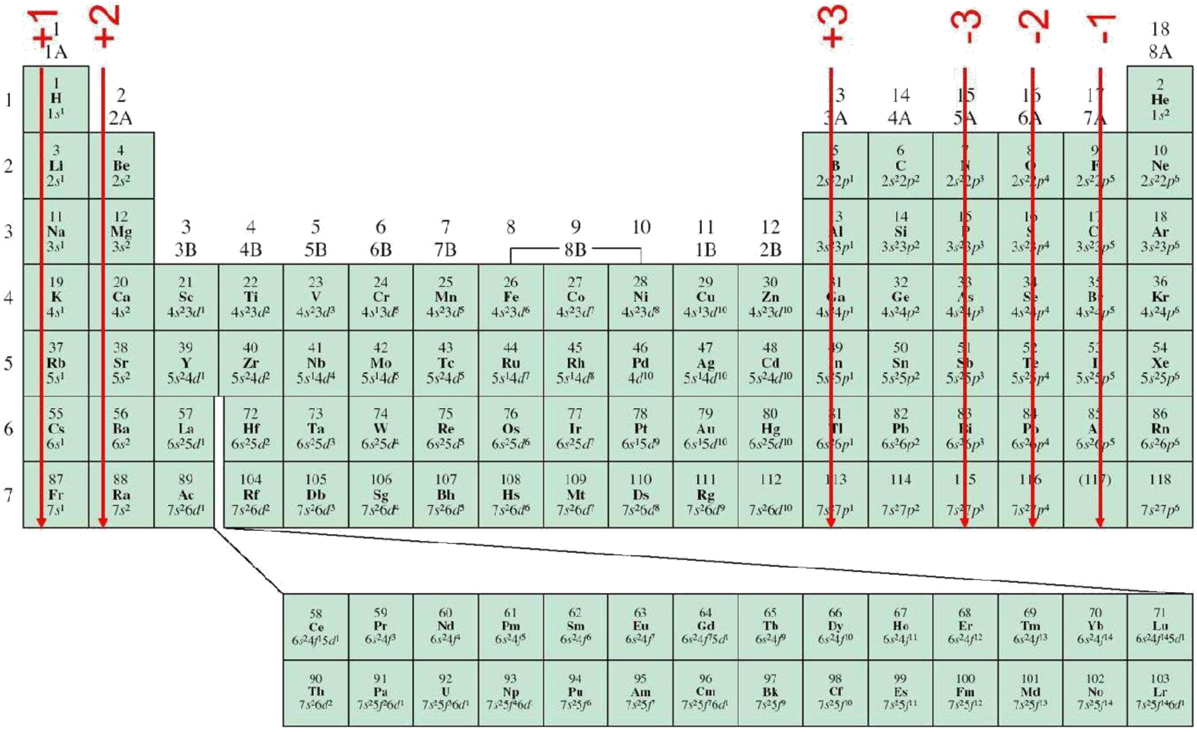
Electron configuration of cations and anions



Ions (cation and anion) of Representative Elements

Cation of Transition Metals

Cations and Anions Of Representative Elements



Ions of Representative Elements

Cation

Na: [Ne]$3s^1$	Na^+: [Ne]
Ca: [Ar]$4s^2$	Ca^{2+}: [Ar]
Al: [Ne]$3s^23p^1$	Al^{3+} : [Ne]

Atoms **lose e-** so that **cation** has a noble-gas outer e- configuration (***ns^2np^6***)

Anion

H: $1s^1$	H^- :$1s^2$ or [He]
F: $1s^22s^22p^5$	F^- :$1s^22s^22p^6$ or [Ne]
O: $1s^22s^22p^4$	O^{2-} :$1s^22s^22p^6$ or [Ne]
N: $1s^22s^22p^3$	N^{3-} :$1s^22s^22p^6$ or [Ne]

Atoms **gain e-** so that **anion** has a noble-gas outer e- configuration (***ns^2np^6***)

Electron Configurations of Cations of Transition Metals

not always isoelectronic with a noble gas

When a cation is formed from an atom of a transition metal, electrons are always removed first from the *ns* orbital and then from the $(n-1)d$ orbitals.

e- are lost from outermost *s orbitals FIRST*

because d orbitals are more stable than the s orbitals in the ionic form of the transition elements.

Fe: $[Ar]4s^2 3d^6$

Fe^{2+}: $[Ar]4s^0 3d^6$ or $[Ar]3d^6$

Fe^{3+}: $[Ar]4s^0 3d^5$ or $[Ar]3d^5$

Mn: $[Ar]4s^2 3d^5$

Mn^{2+}: $[Ar]4s^0 3d^5$ or $[Ar]3d^5$

Isoelectronic

Ions or atoms that have the same number of electrons, and hence the same electron configuration

Na^+: [Ne]

Al^{3+}: [Ne]

O^{2-}: $1s^2 2s^2 2p^6$ or [Ne]

F^-: $1s^2 2s^2 2p^6$ or [Ne]

N^{3-}: $1s^2 2s^2 2p^6$ or [Ne]

Na^+, Al^{3+}, F^-, O^{2-}, and N^{3-} are all ***isoelectronic*** with Ne

What neutral atom is isoelectronic with H^- ?

H^-: $1s^2$ same electron configuration as He

8.2 Periodic Variation In Physical Properties

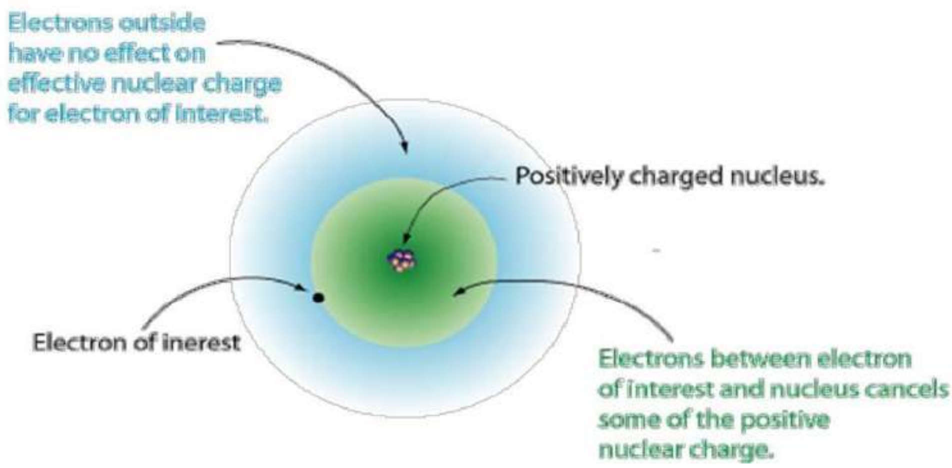
Periodic trends

Many trends in physical and chemical properties can be explained by e- configuration

1) Effective nuclear change
2) Atomic radius
3) Ionic radius
4) Ionization energy
5) Electron affinity

Effective nuclear charge (Z_{eff}) is the net "positive charge" that an e- experiences from nucleus.

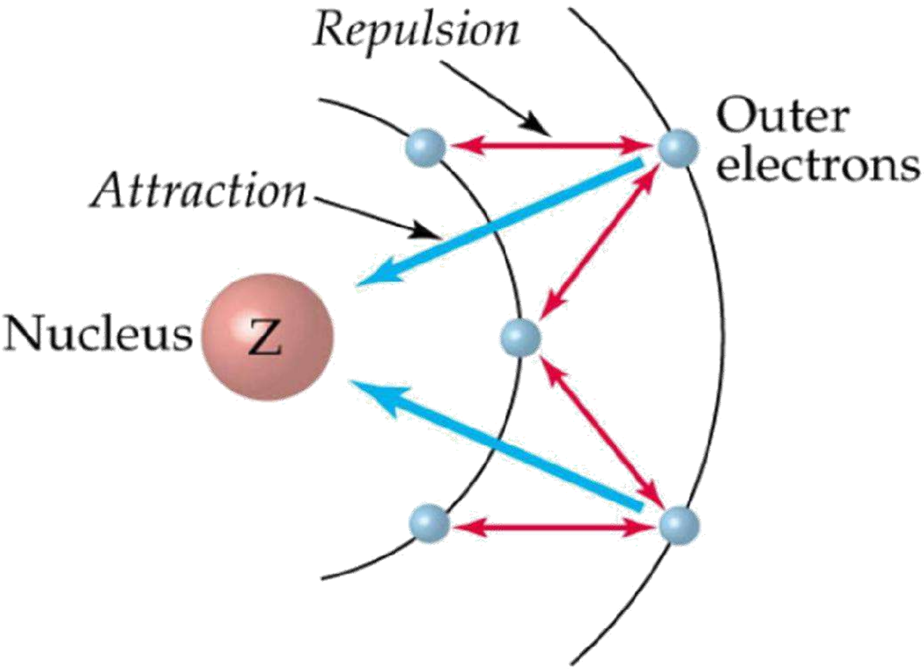
- inner e- shield outer/valence e- from nucleus
- lower effective charge on nucleus
- shielding effect of e- reduces the attraction between the nucleus and the e-



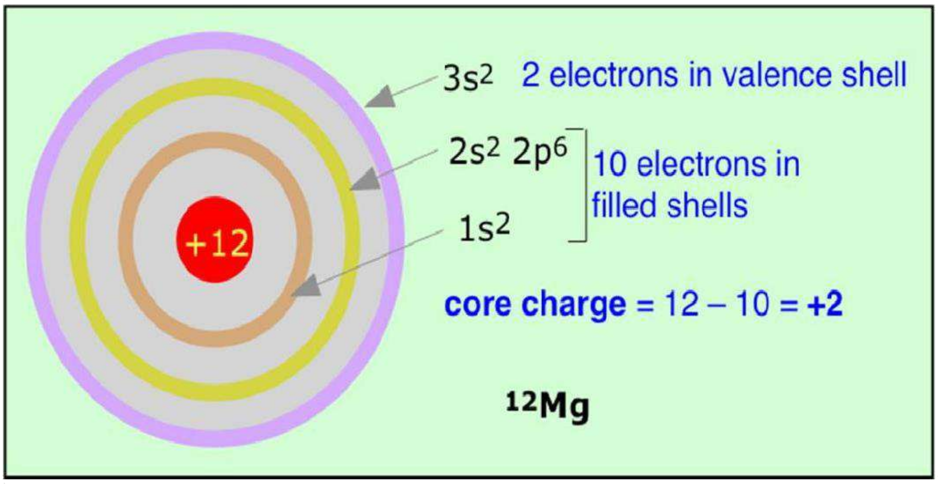
Effective Nuclear Charge

= Actual Nuclear Charge - Shielding Effect

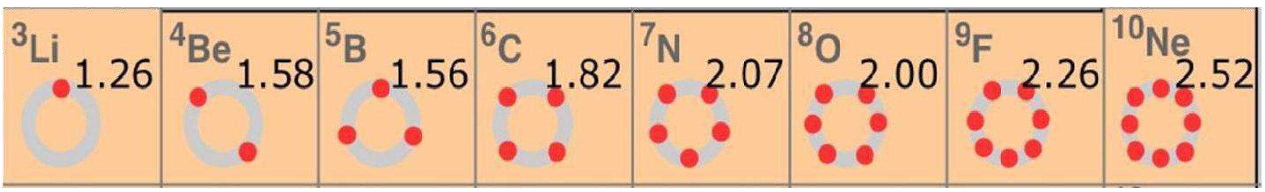
= *Z* (number of proton) - number of inner/core electrons

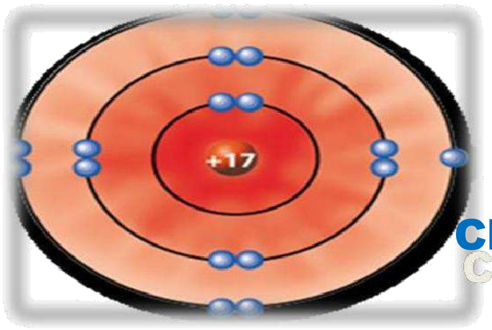


	Z	Core	Z_{eff}
Na	11	10	1
Mg	12	10	2
Al	13	10	3
Si	14	10	4



$Z_{eff} = Z$ (number of proton)– number of inner or core electrons





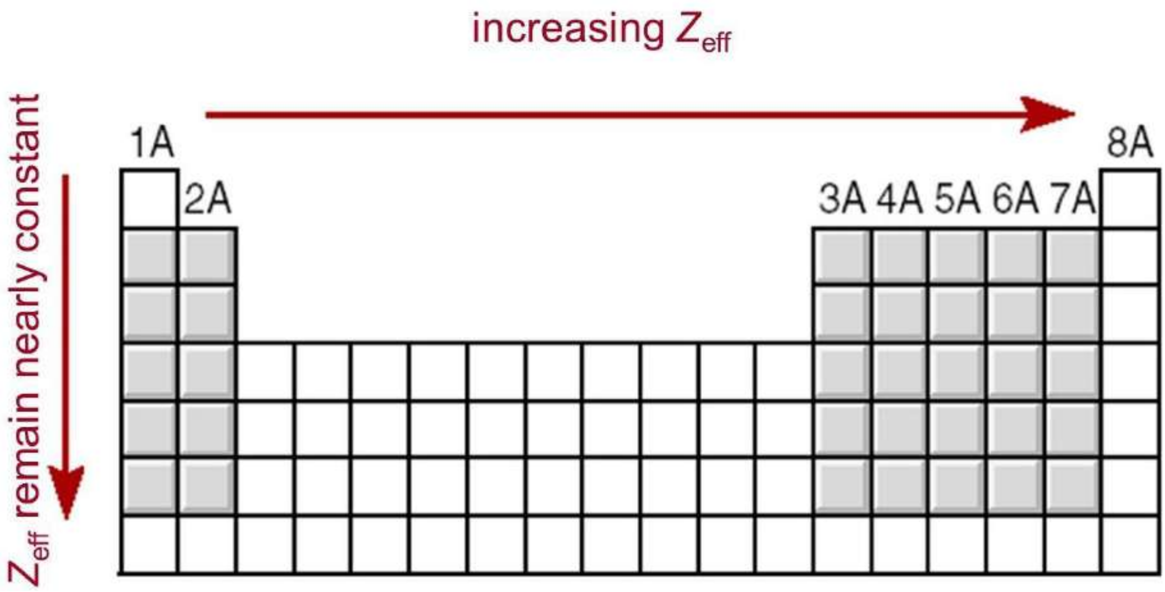
Chlorine
Chlorine

+17 Actual nuclear charge
+17 Actual nuclear charge

-10 Inner shell electrons
-10 Inner shell electrons

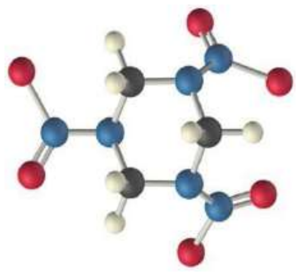
+7 Effective nuclear charge
+7 Effective nuclear charge

Effective Nuclear Charge (Z_{eff})



LECTURE 9

Chemical Bonding I: Basic Concepts

9.1 lewis Dot Symbols

9.2 The Ionic bond

9.3 The Covalent bond

9.4 Electroegativity

9.5 Writing Lewis Structures

9.6 Formal Charge and Lewis Structures

9.7 The Concept of Resonance

9.8 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.**

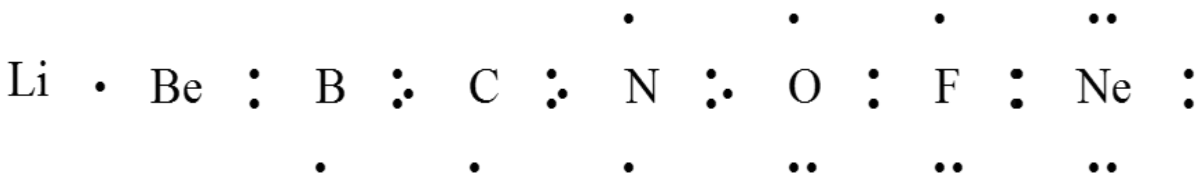
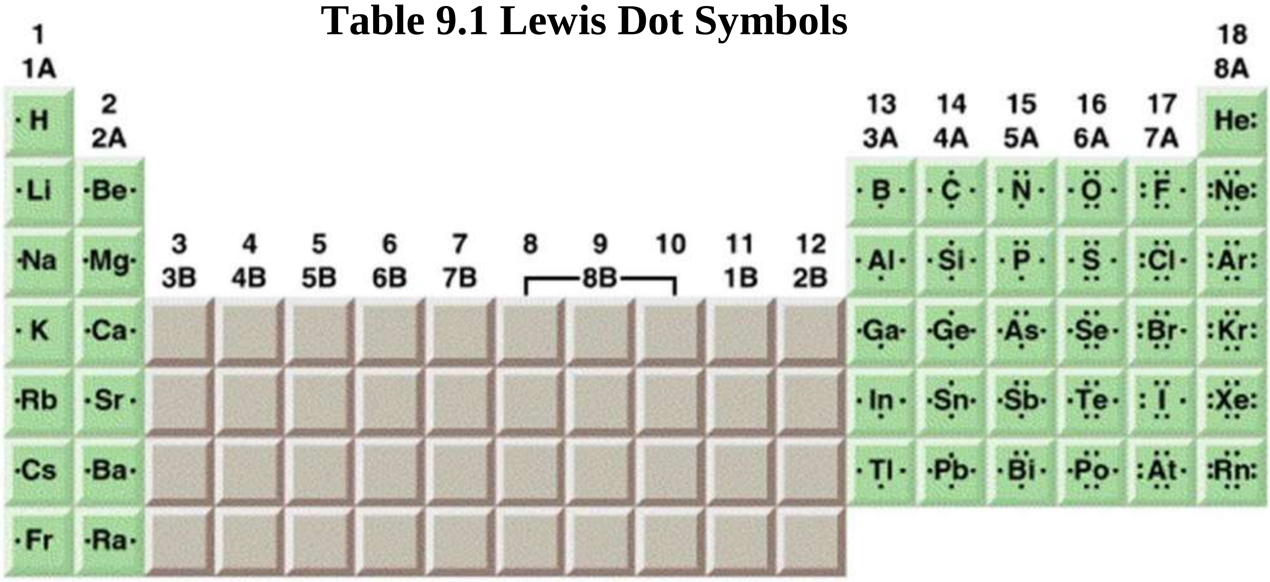


Table 9.1 Lewis Dot Symbols

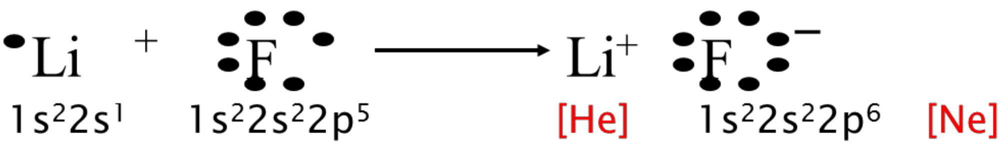


Types of Bonds

Types of Atoms	Type of Bond	Bond Characteristic
metals to nonmetals	Ionic	electrons transferred
nonmetals to nonmetals	Covalent	electrons 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.

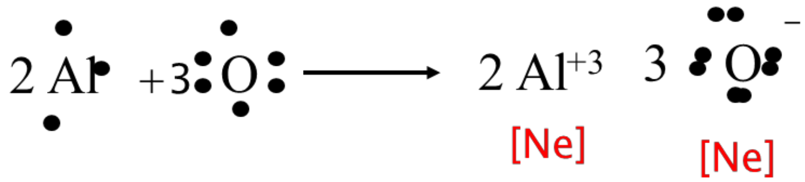
Note: Do not show the charges in the final product.

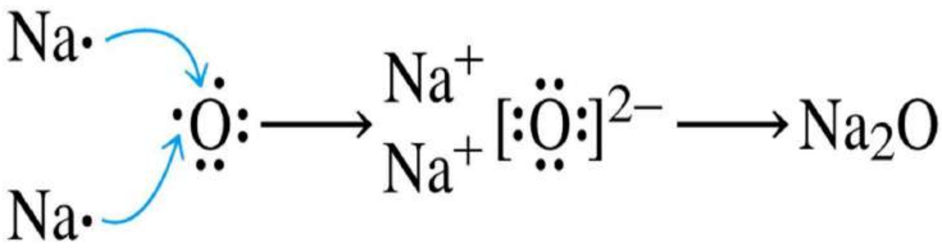
Example: KI NOT K+I-

Example: Ba+2 & F- - Need two negatives to neutralize +2 charge on barium ion: Ba+2 F-1 F-1 = BaF2

Example 9.1

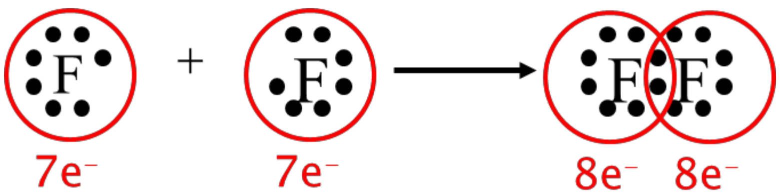
Use Lewis dot symbol to show formation of Al2O3



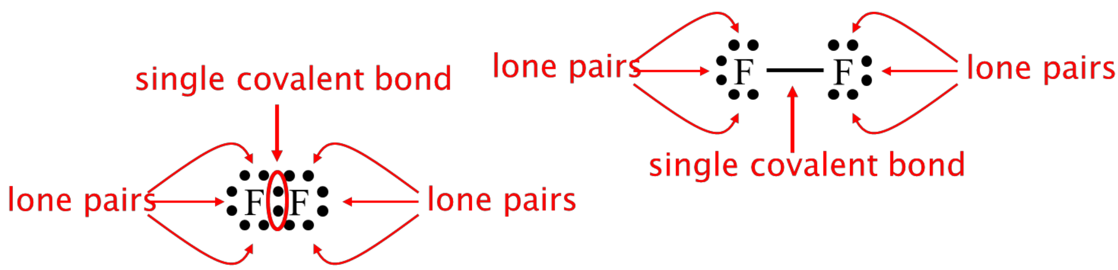


9.3 The Covalent Bond

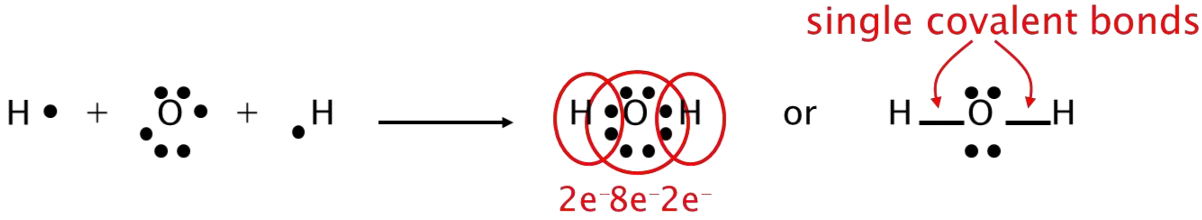
- A covalent bond is a chemical bond in which two or more electrons are shared by two atoms.



Lewis structure of F_2

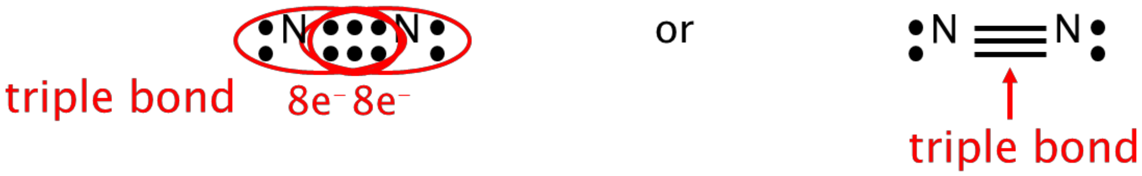


Lewis structure of water

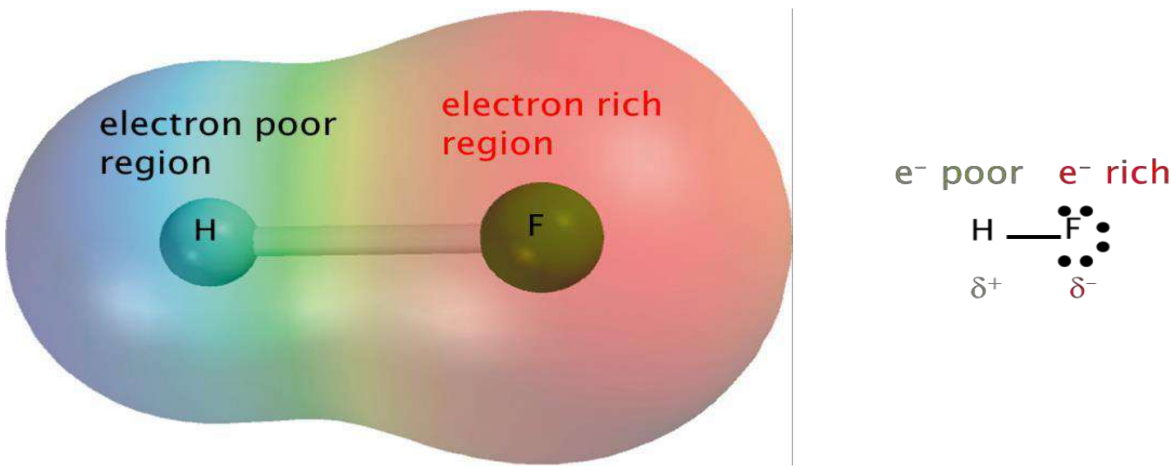


Double bond – two atoms share **two pairs** of electrons

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.

9.4 Electronegativity

- Electronegativity is the ability of an atom to attract toward itself the electrons in a chemical bond.
- High electronegativity →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 from pure covelent bond (H2).

The Electronegativities of Common Elements

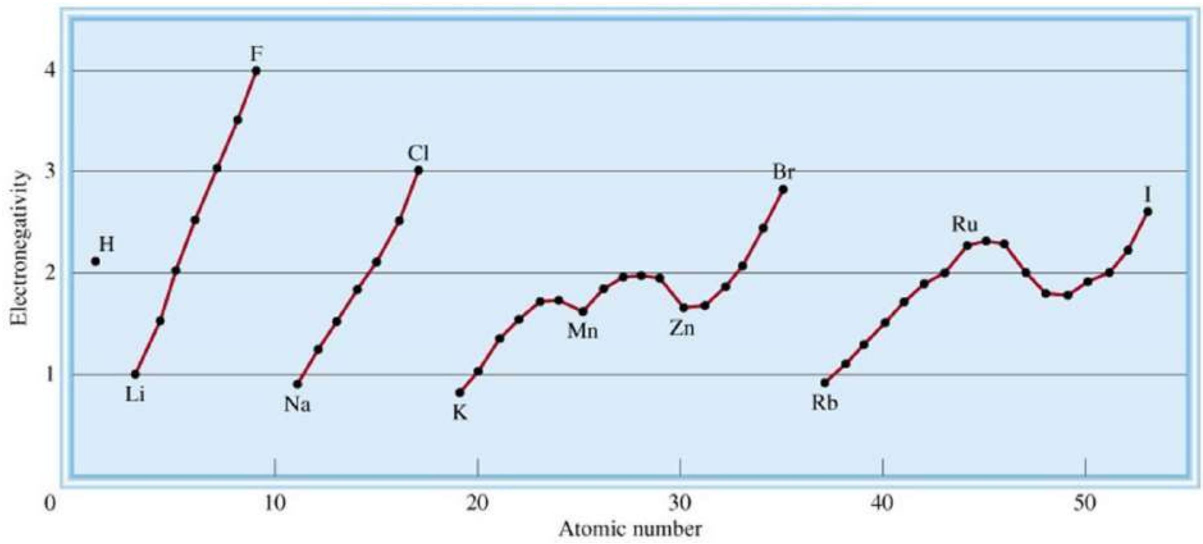
Increasing electronegativity (left to right across a period; bottom to top within a group)

1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
H 2.1																	
Li 1.0	**Be** 1.5											**B** 2.0	**C** 2.5	**N** 3.0	**O** 3.5	**F** 4.0	
Na 0.9	**Mg** 1.2											**Al** 1.5	**Si** 1.8	**P** 2.1	**S** 2.5	**Cl** 3.0	
K 0.8	**Ca** 1.0	**Sc** 1.3	**Ti** 1.5	**V** 1.6	**Cr** 1.6	**Mn** 1.5	**Fe** 1.8	**Co** 1.9	**Ni** 1.9	**Cu** 1.9	**Zn** 1.6	**Ga** 1.6	**Ge** 1.8	**As** 2.0	**Se** 2.4	**Br** 2.8	**Kr** 3.0
Rb 0.8	**Sr** 1.0	**Y** 1.2	**Zr** 1.4	**Nb** 1.6	**Mo** 1.8	**Tc** 1.9	**Ru** 2.2	**Rh** 2.2	**Pd** 2.2	**Ag** 1.9	**Cd** 1.7	**In** 1.7	**Sn** 1.8	**Sb** 1.9	**Te** 2.1	**I** 2.5	**Xe** 2.6
Cs 0.7	**Ba** 0.9	**La-Lu** 1.0-1.2	**Hf** 1.3	**Ta** 1.5	**W** 1.7	**Re** 1.9	**Os** 2.2	**Ir** 2.2	**Pt** 2.2	**Au** 2.4	**Hg** 1.9	**Tl** 1.8	**Pb** 1.9	**Bi** 1.9	**Po** 2.0	**At** 2.2	
Fr 0.7	**Ra** 0.9																

- **Electron Affinity** (EA) and electronegativity are related but in different concept
- (EA) refers to isolated atoms attraction for additional electron (experimental)
- EA →measurable, Cl is highest

- **Electronegativity** signifies the ability of an atom in a chemical bond(with another atom) to attract the shared electrons (estimated)
- Electronegativity - relative, F is highest

Variation of Electronegativity with Atomic Number



Example 9.2

- 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
  Ionic
- c) C−C =2.5−2.5=0
  covalent

- Classify the following bonds as ionic, polar covalent, or covalent
- A) CsCl =3−1=2
  Ionic
- b) H_2S =2.5−2.1=0.4
  Polar covalent
- c) N−N =3−3=0
  covalent

9.5 Writing Lewis structures

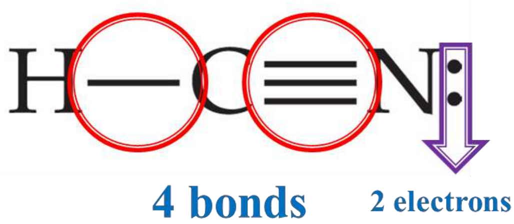
1. Write the skeletal structure of the compounds, using chemical symbol and placing bonded atoms next to one another.

- 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=B-C.

Writing Lewis Structures



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

B = 1X2+8X1+8X1 =18electrons

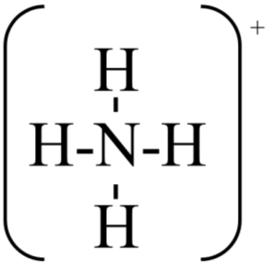
C = 18-10 =8/2=4 bonds

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

NH4+

- **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= 8-4 =4 non bonding electrons , 2 pair of electrons**



Example 9.3

Write the Lewis structure of nitrogen trifluoride (NF_3).

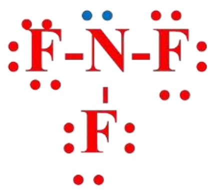
Step 1 – N is less electronegative than F, put N in center

Step 2 – A= 5X1 + 7X3 = 26 valance electrons

Step 3 – B = 8X1+8X3 =32 electrons

Step 4 – C = 32-26 =6/2=3 bonds

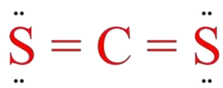
Step 5 – D= 26-6 =20 nonbonding electrons or 10 pair of electrons



Example 9.3

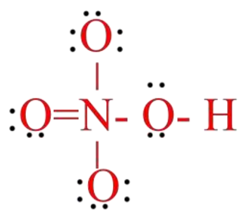
Write the Lewis structure of carbon disulfide (CS2).

- 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



Example 9.4

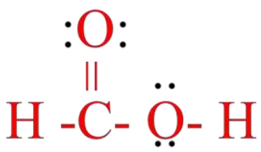
- Write the Lewis structure for nitric acid (HNO3) in which the three O atoms are bonded to the central N atom and ionizable H atom is bonded to one of the O atom.
- Step 1 –put N in center ,surrounded by 3O atoms , H bonded to one of the O
- Step 2 – Count valence electrons 5 + (3 x 6) +1 = 24 nonbonding electrons or 12 pair of electrons.



Example 9.4

Write the Lewis structure of formic acid (HCOOH).

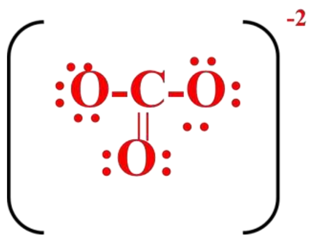
- Step 1 –put C in center ,surrounded by 2O atoms , H Step 2 – A= 4X1 + 6X2 +2x1 = 18 valance electrons
- Step 3 – B = 8X1+8X2 +2 x2 =28 electrons
- Step 4 - C = 28-18 =10/2=5 bonds
- Step 5 - D= 18-10 =8 nonbonding electrons or 4 pair of electrons



Example 9.5

Write the Lewis structure of carbon dioxide [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



Example 9.5

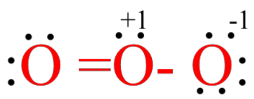
Write the Lewis structure of carbon dioxide [NO2]-1

- 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 =6/2=3 bonds
- Step 5 - D= 18-6 =12 nonbonding electrons or 6 pair of electrons

9.6 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.

$$\text{formal charge on an atom in a Lewis structure} = \text{total number of valence electrons in the free atom} - \text{total number of nonbonding electrons} - \frac{1}{2}\left(\text{total number of bonding electrons}\right)$$

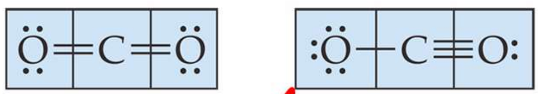


6	6	6
6	5	7
0	+1	-1

- 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

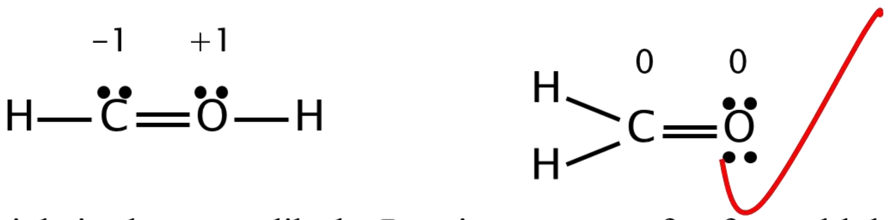
formal charge and Lewis structures

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.



	O	C	O	O	C	O
Valence electrons:	6	4	6	6	4	6
−(Electrons assigned to atom):	6	4	6	7	4	5
Formal charge:	0	0	0	−1	0	+1

Which is the most likely Lewis structure for formaldehyde CH_2O

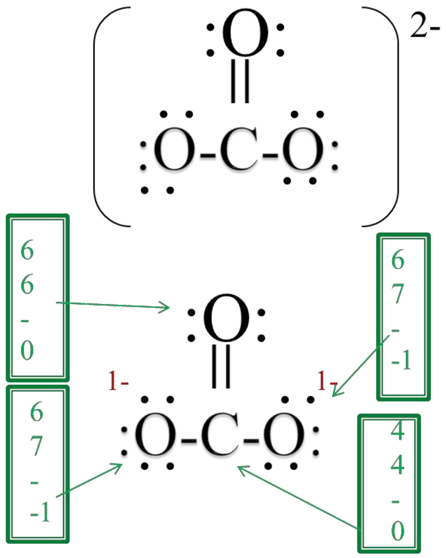


Which is the most likely Lewis structure for formaldehyde C,H,N

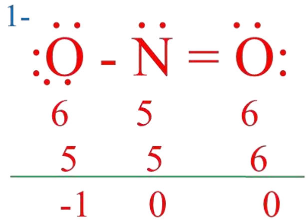
H-C≡N:

Example 9.6

Write the formal charge for the carbonate ion?

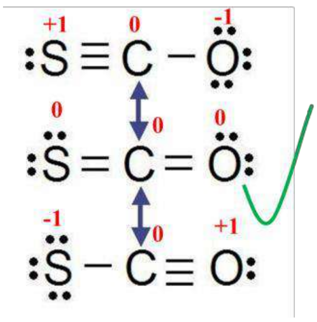


Write the formal charge for the NO_2^- ion?

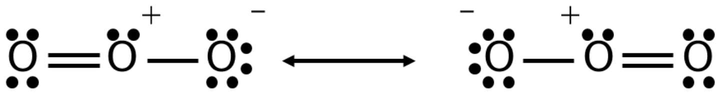


9.7 the concept of resonance

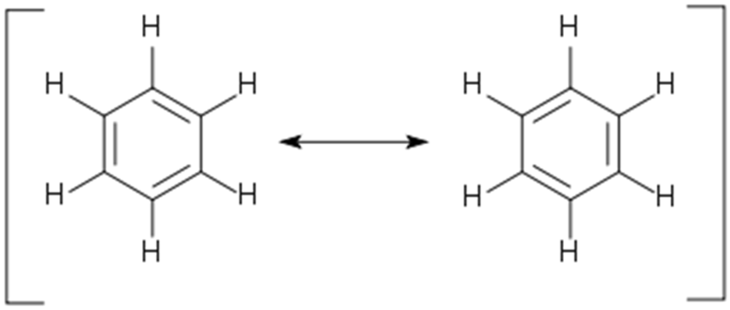
- A resonance structure is one of two or more Lewis structures for a single molecule that cannot be represented accurately by only one Lewis structure (after formal charge has been determined).
- More possible structures gives the overall structure more validity.



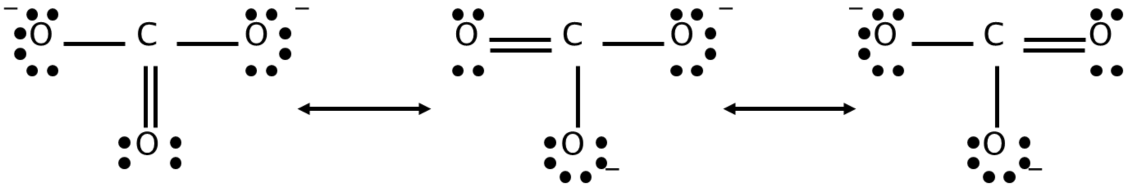
Ozone



Benzene

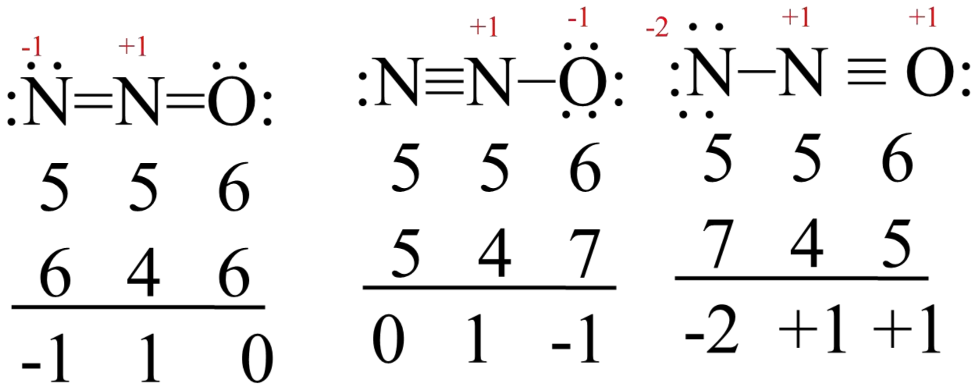


What are the resonance structures of the carbonate (CO_3^{2-}) ion?



Example 9.8

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



B> A > C

9.8 the exception of octate rules

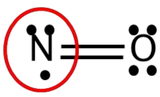
- There are three types of ions or molecules that do not follow the octet rule:
-
- Ions or molecules with an odd number of electrons
- Ions or molecules with less than an octet (the incomplete Octet)
- Ions or molecules with more than eight valence electrons (an expanded octet)

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 – $6e^-$
$11e^-$

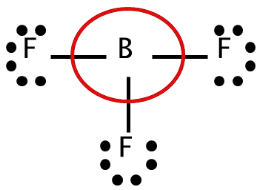


The incomplete Octet

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

BF_3

B – $3e^-$
3F – $3x7e^-$
$24e^-$



3 single bonds (3x2) = 6
9 lone pairs (9x2) = 18
Total = 24

BeH_2

Be – $2e^-$
2H – $2x1e^-$
$4e^-$

An expanded octet

- Usually occurs in element in 3rd period and beyond

  More than 4 bonds

- Elements ≥ row 3 can use s, p & d orbitals and have > 8 VE
- P: 8 OR 10
- S: 8, 10, OR 12
- Xe: 8, 10, OR 12

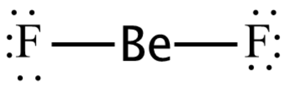
Examples

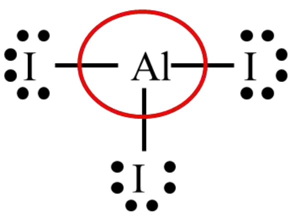
SF6 PF5 XeF4

Example 9.9

Write Lewis structure AlI_3

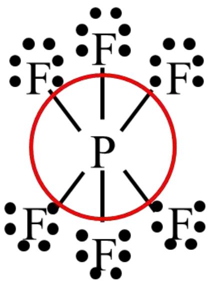
Write Lewis structure BeF_2

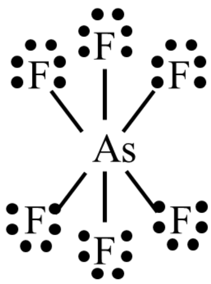




Example 9.10

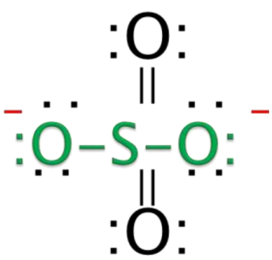
Write Lewis structure PF_5 Write Lewis structure AsF_5

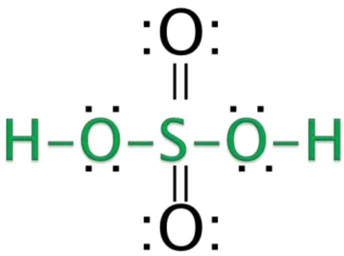




Example 9.11

Write Lewis structure $[SO_4]^{-2}$ Write Lewis structure H_2SO_4





Lecture References :

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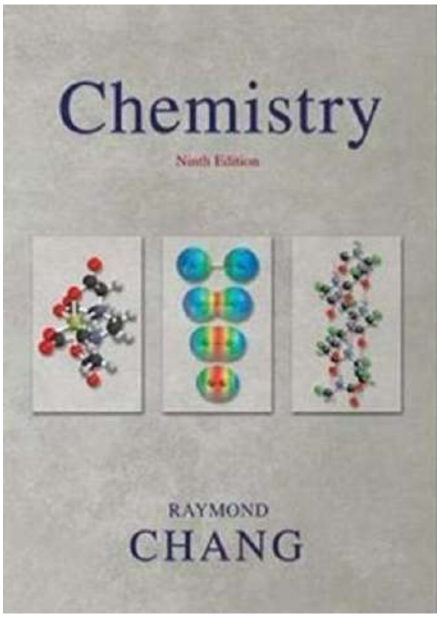

2. Essentials of General Chemistry By D.D.Ebbing, S.D.Gammon,andR.O.Ragsdale,2003 , Houghton Mifflin Company,New York.