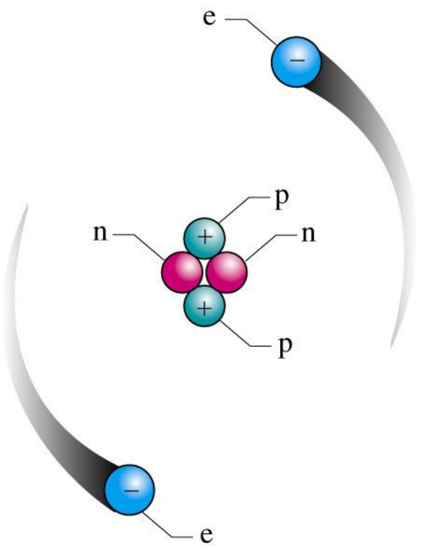


Chapter 2: Atoms and the Atomic Theory

Contents

Contents

2-1 Early Discoveries and the Atomic Theory

- Lavoisier 1774: Law of conservation of mass

"The total mass of substances present after a chemical reaction is the same as the total mass of substances before the reaction."

- Proust 1799: Law of constant composition

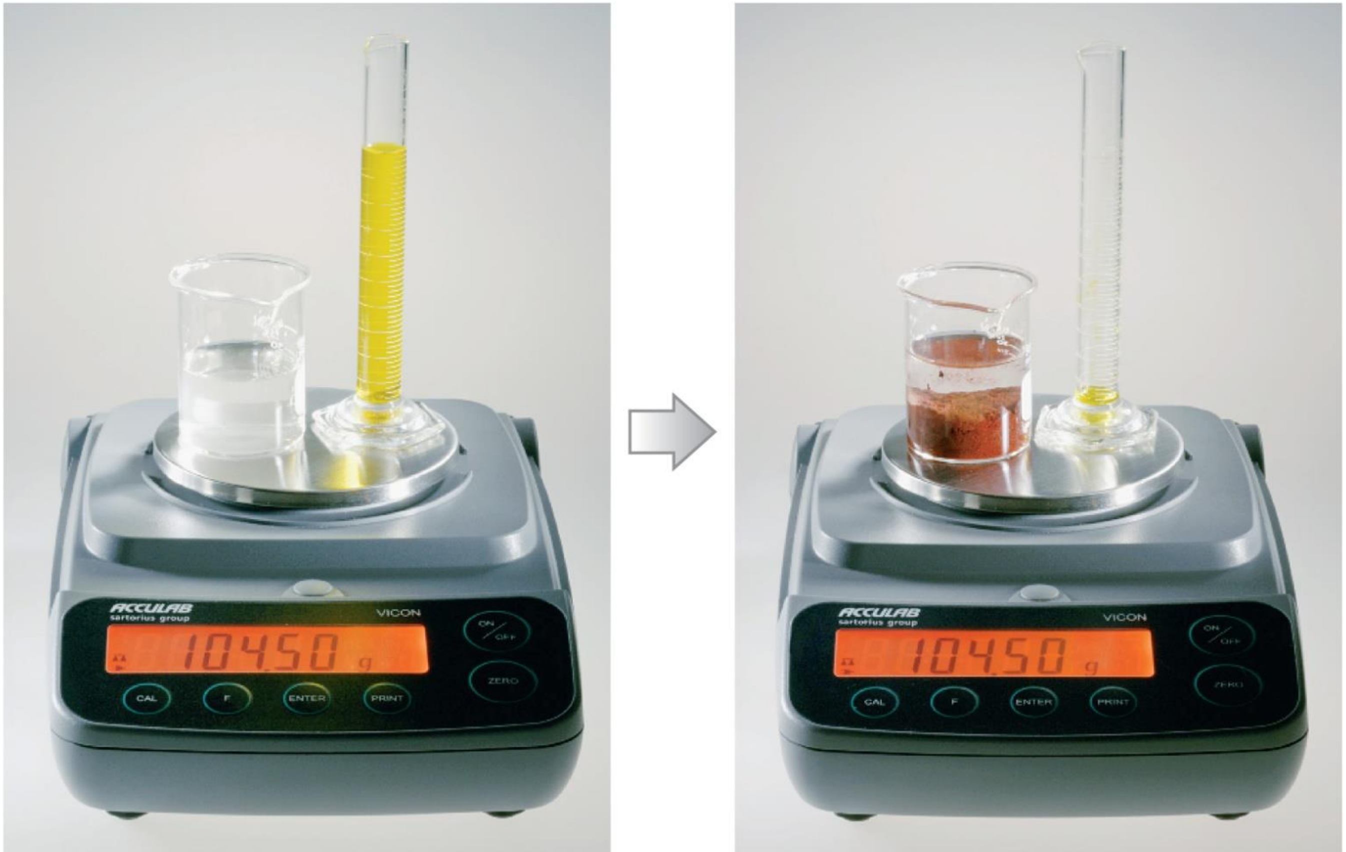
"All samples of a compound have the same composition the same proportions by mass of the constituent elements."

- Dalton 1803-1888: Atomic Theory

"If two elements form more than a single compound, the masses of one element combined with a fixed mass of the second are in the ratio of small whole numbers."

▲ FIGURE 2-1
Two combustion reactions
The apparent product of the combustion of the match—the ash—weighs *less* than the match. The product of the combustion of the magnesium ribbon (the "smoke") weighs *more* than the ribbon. Actually, in each case, the total mass remains unchanged. To understand this, you have to know that oxygen gas enters into both combustions and that water and carbon dioxide are also products of the combustion of the match.

Conservation of Mass



(a) (b)

Dalton's Atomic Theory

① Each element is composed of small particles called **atoms**.

② Atoms are **neither created nor destroyed** in chemical reactions.

③ All atoms of a given element are **identical.**

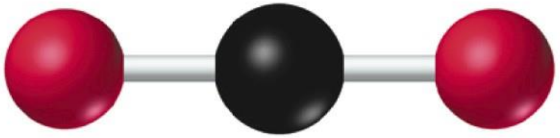
④ **Compounds** are formed when atoms of **more than one element** combine.

Consequences of Dalton's theory

- **Law of Definite Proportions: combinations of elements are in ratios of small whole numbers.**

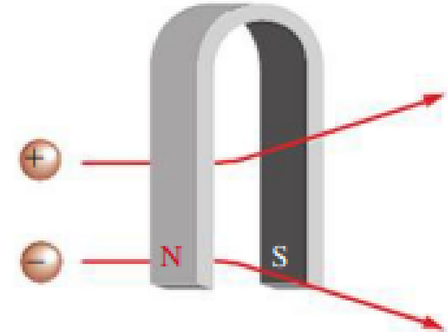
☆ **In forming carbon monoxide, 1.33 g of oxygen combines with 1.0 g of carbon.**

☆ **In the formation of carbon dioxide 2.66 g of oxygen combines with 1.0 g of carbon.**



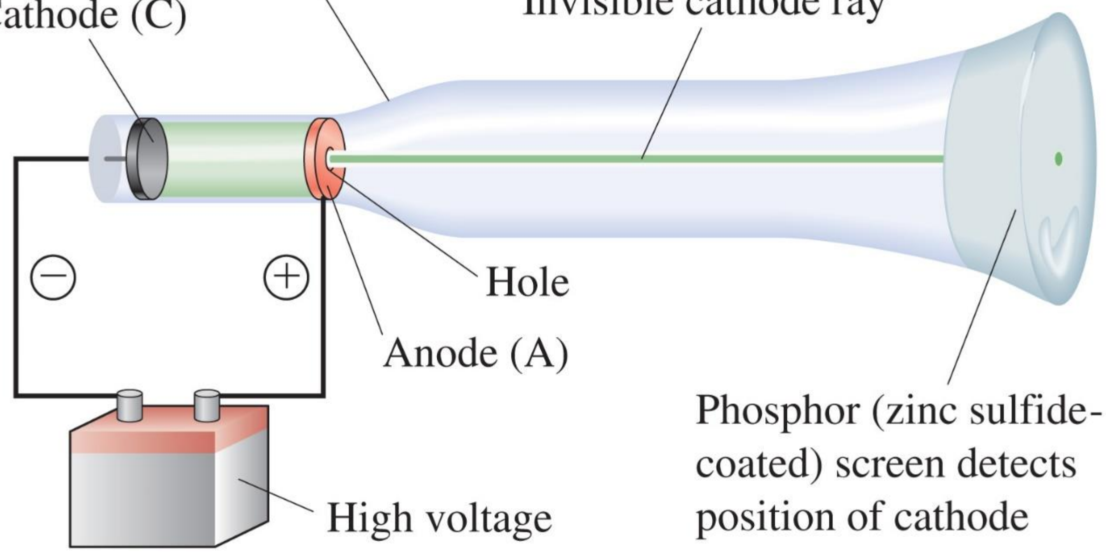
2-2 Electrons and Other Discoveries in Atomic Physics

▲ FIGURE 2-4
Forces between electrically charged objects
(a) Electrostatically charged comb. If you comb your hair on a dry day, a static charge develops on the comb and causes bits of paper to be attracted to the comb. **(b)** Both objects on the left carry a negative electric charge. Objects with like charge repel each other. The objects in the center lack any electric charge and exert no forces on each other. The objects on the right carry opposite charges—one positive and one negative—and attract each other.



▲ FIGURE 2-5
Effect of a magnetic field on charged particles
When charged particles travel through a magnetic field so that their path is perpendicular to the field, they are deflected by the field. Negatively charged particles are deflected in one direction, and positively charged particles in the opposite direction. Several phenomena described in this section depend on this behavior.

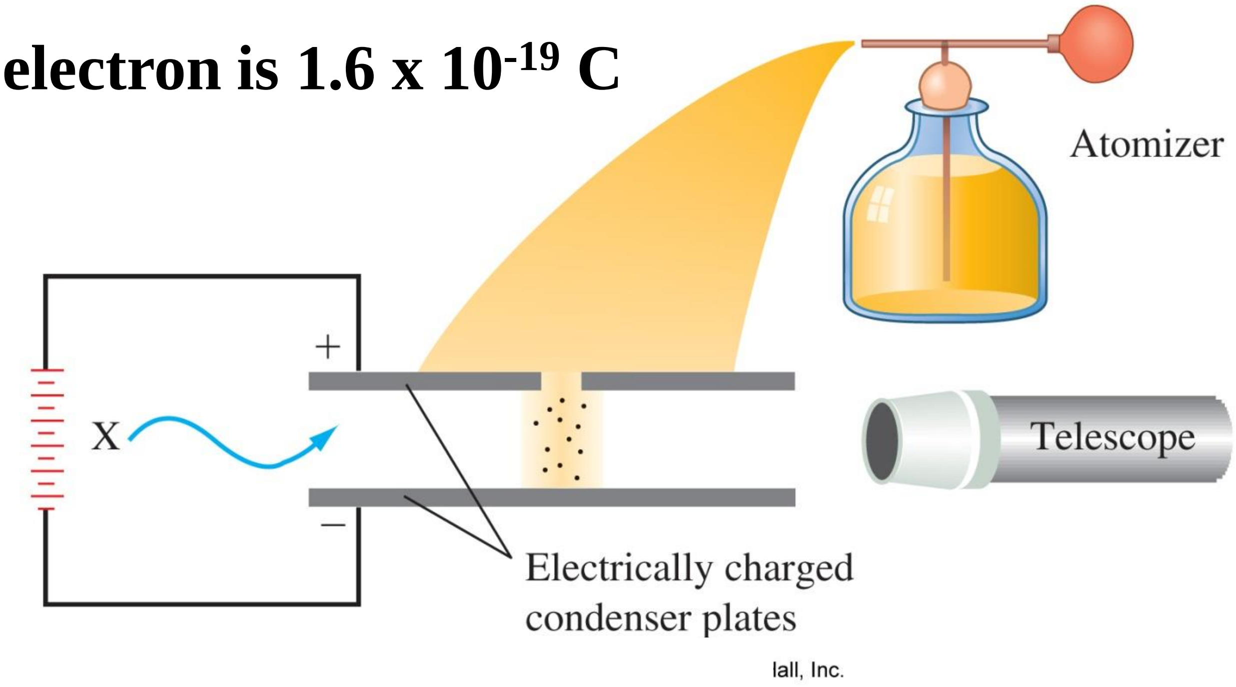
Cathode ray tube



◀ FIGURE 2-6
A cathode-ray tube
The high-voltage source of electricity creates a negative charge on the electrode at the left (cathode) and a positive charge on the electrode at the right (anode). Cathode rays pass from the cathode (C) to the anode (A), which is perforated to allow the passage of a narrow beam of cathode rays. The rays are visible only through the green fluorescence that they produce on the zinc sulfide–coated screen at the end of the tube. They are invisible in other parts of the tube.

Charge on the electron

The charge of an electron is 1.6 x 10^{-19} C



- ☆ From 1906-1914 Robert Millikan showed ionized oil drops can be balanced against the pull of gravity by an electric field.
- ☆The charge is an *integral* multiple of the electronic charge, *e*.

Radioactivity

Radioactivity is the spontaneous emission of radiation from a substance.

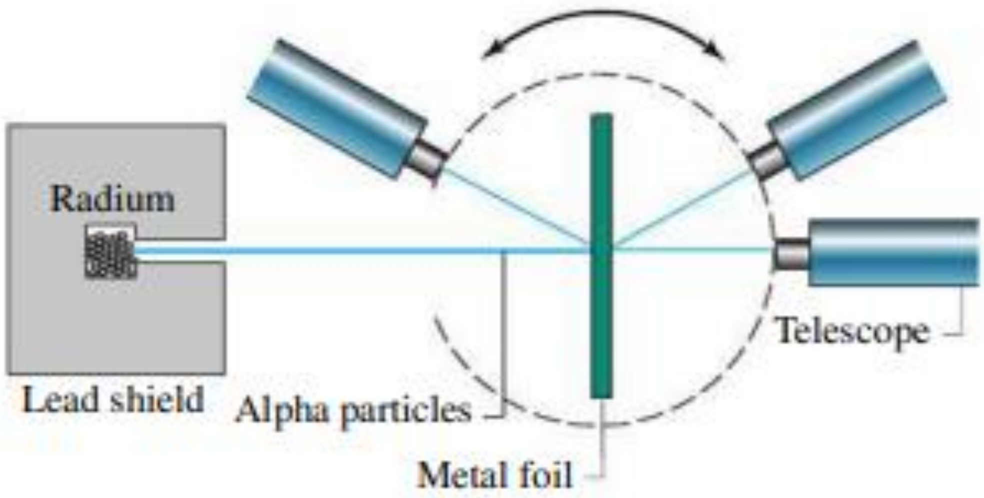
- ☆ X-rays and γ-rays are high-energy light.
- ☆ α-particles are a stream of helium nuclei, He^{2+}.
- ☆ β-particles are a stream of high speed electrons that originate in the nucleus.

2-3 The Nuclear Atom

Geiger and Rutherford 1909

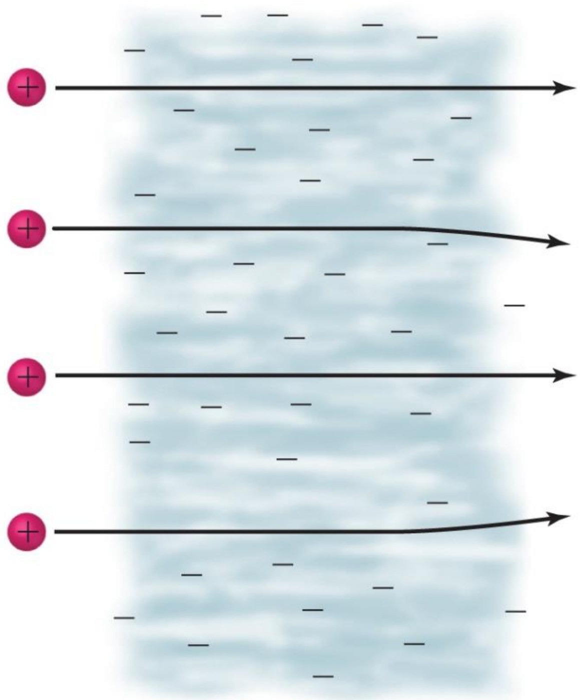
He based his explanation on a model of the atom known as the nuclear atom and having these features:

1. Most of the mass and all of the positive charge of an atom are centered in a very small region called the nucleus. The remainder of the atom is mostly empty space.
2. The magnitude of the positive charge is different for different atoms and is approximately one-half the atomic weight of the element.
3. There are as many electrons outside the nucleus as there are units of positive charge on the nucleus. The atom as a whole is electrically neutral.

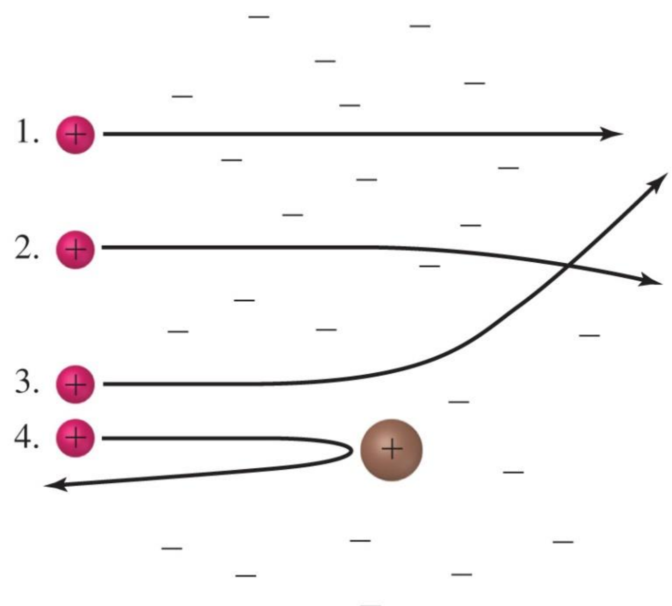


▶ FIGURE 2-11
The scattering of α particles by metal foil
The telescope travels in a circular track around an evacuated chamber containing the metal foil. Most α particles pass through the metal foil undeflected, but some are deflected through large angles.

The α-particle experiment



- Most of the mass and all of the positive charge is concentrated in a small region called the nucleus .



- There are as many electrons outside the nucleus as there are units of positive charge on the nucleus

Nuclear Structure

Atomic Diameter **10^{-8} cm**

1 Å

Nuclear diameter **10^{-13} cm**

Particle	Mass		Electric Charge	
	kg	**amu**	**Coulombs**	**(*e*)**
Electron	9.1094×10^{-31}	0.00054858	-1.6022×10^{-19}	–1
Proton	1.6726×10^{-27}	1.0073	$+1.6022 \times 10^{-19}$	+1
Neutron	1.6749×10^{-27}	1.0087	0	0

amu*:atomic mass unit

Scale of Atoms

∗The heaviest atom has a mass of only 4.8×10^{-22} g and a diameter of only 5×10^{-10} m.

<u>Useful units:</u>

- ☆ **1 amu (atomic mass unit) = 1.66054×10^{-24} g**
- ☆ **1 pm (picometer) = 1×10^{-12} m**
- ☆ **1 Å (Angstrom) = 1×10^{-10} m = 100 pm = 1×10^{-8} cm**

Biggest atom is 240 amu and is 50 **Å** across.
Typical C-C bond length 154 pm (1.54 **Å**)
Molecular models are 1 **Å** /inch or about 0.4 **Å** /cm

2-4 Chemical Elements

∗To represent a particular atom we use symbolism:

$$\text{number p} + \text{number n} \rightarrow A$$

$$\text{number p} \rightarrow Z$$

$${}^{A}_{Z}\mathrm{E}^{\pm ?} \longleftarrow \text{number p} - \text{number e}$$

A= mass number Z = atomic number

2-5 Atomic Mass

$$\begin{matrix}\text{at. mass}\\ \text{of an}\\ \text{element}\end{matrix} = \left(\begin{matrix}\text{fractional}\\ \text{abundance of}\\ \text{isotope 1}\end{matrix} \times \begin{matrix}\text{mass of}\\ \text{isotope 1}\end{matrix}\right) + \left(\begin{matrix}\text{fractional}\\ \text{abundance of}\\ \text{isotope 2}\end{matrix} \times \begin{matrix}\text{mass of}\\ \text{isotope 2}\end{matrix}\right) + \ldots \quad \textbf{(2.3)}$$

$$\begin{aligned}\begin{matrix}\text{at. mass of naturally}\\ \text{occurring carbon}\end{matrix} &= 0.9893 \times 12\text{ u} + (1 - 0.9893) \times 13.0033548378\text{ u}\\ &= 13.0033548378\text{ u} - 0.9893 \times (13.0033548378\text{ u} - 12\text{ u})\\ &= 13.0033548378\text{ u} - 0.9893 \times (1.0033548378\text{ u})\\ &= 13.0033548378\text{ u} - 0.9893\\ &= 12.0107\text{ u}\end{aligned}$$

2-5 Atomic Mass

98,992 atoms of C^{12}_{6} (12 u exactly)

$+$

1,108 atoms of C^{13}_{6} (13.00335 u)

$\downarrow$

100,000 atoms of naturally occurring C (12.011 u)

EXAMPLE 2-6

Relating the Masses and Natural Abundances of Isotopes to the Atomic Mass of an Element. Bromine has two naturally occurring isotopes. One of them, bromine-79 was a mass of 78.9183 u and an abundance of 50.69%. What must be the mass and percent natural abundance of the other, bromine-81?

What do we know:

The sum of the percent natural abundances must be 100%.

The average mass of bromine (read from the periodic table) is the weighted contribution of the percent abundance times the mass of each contributing isotope. Recall equation 2.3.

EXAMPLE 2-6

Strategy

Identify the unknown abundance of bromine-81 by calculation. Use this value in the equation for the average mass of an element to solve for the mass of the unknown isotope. Recall equation 2.3.

Solution

Write the general equations

$$100\% = \chi_1 + \chi_2 + \chi_3 \ldots$$

$$\text{Atomic mass} = \chi_1 \times m_1 + \chi_2 \times m_2 + \chi_3 \times m_3 \ldots$$

EXAMPLE 2-6

Identify the knowns and unknowns in the specific equations

$$\text{Atomic mass} = \chi_{Br\text{-}79} \times m_{Br\text{-}79} + \chi_{Br\text{-}81} \times m_{Br\text{-}81}$$

Solve

$$100\% = \chi_{79} + \chi_{81}$$

$$\chi_{81} = 100\% - \chi_{79}$$

$$m_{Br\text{-}81} = \frac{\text{Atomic mass} - (\chi_{Br\text{-}79} \times m_{Br\text{-}79})}{\chi_{Br\text{-}81}}$$

EXAMPLE 2-6

Calculate

$$m_{Br\text{-}81} = \frac{79.904\ \text{u} - (0.5069 \times 78.9183\ \text{u})}{0.4931} = 80.92\ \text{u}$$

Key Concepts

- An element is a substance made up of only one type of atom.
- The atomic number of an atom is equal to the number of protons in its nucleus.
- The number of electrons surrounding the nucleus of an atom is equal to the number of protons in its nucleus.
- Different atoms of the same element can have a different number of neutrons.
- Atoms of the same element with different numbers of neutrons are called "isotopes" of that element.
- The atomic mass of an element is the average mass of the different isotopes of the element.
- The atoms in the periodic table are arranged to show characteristics and relationships between atoms and groups of atoms.
- The periodic table is a chart containing information about the atoms that make up all matter.

The Periodic table

Alkali Metals

Alkaline Earths

Transition Metals

Halogens

Main Group

Noble Gases

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H 1.00794																	2 He 4.00260
3 Li 6.941	4 Be 9.01218											5 B 10.811	6 C 12.011	7 N 14.0067	8 O 15.9994	9 F 18.9984	10 Ne 20.1797
11 Na 22.9898	12 Mg 24.3050											13 Al 26.9815	14 Si 28.0855	15 P 30.9738	16 S 32.06	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.9559	22 Ti 47.88	23 V 50.9415	24 Cr 51.9961	25 Mn 54.9381	26 Fe 55.847	27 Co 58.9332	28 Ni 58.693	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.9216	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224	41 Nb 92.9064	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.906	46 Pd 106.42	47 Ag 107.868	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.757	52 Te 127.60	53 I 126.904	54 Xe 131.29
55 Cs 132.905	56 Ba 137.327	57 *La 138.906	72 Hf 178.49	73 Ta 180.948	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.967	80 Hg 200.59	81 Tl 204.383	82 Pb 207.2	83 Bi 208.980	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.025	89 †Ac 227.028	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 (269)	111 (272)	112 (272)		114 (287)		116 (289)		118 (293)

*Lanthanide series	58 Ce 140.115	59 Pr 140.908	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.965	64 Gd 157.25	65 Tb 158.925	66 Dy 162.50	67 Ho 164.930	68 Er 167.26	69 Tm 168.934	70 Yb 173.04	71 Lu 174.967
†Actinide series	90 Th 232.038	91 Pa 231.036	92 U 238.029	93 Np 237.048	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

Main Group

Lanthanides and Actinides

The Periodic Table

- In the periodic table, elements are listed according to increasing atomic number starting at the upper left and arranged in a series of horizontal rows. This arrangement places similar elements in vertical groups, or families.
- Some of the groups are given distinctive names, mostly related to an important property of the elements in the group.
- For example, the group 17 elements are called the halogens, a term derived from Greek, meaning salt former.

The Periodic Table

- Each element is listed in the periodic table by placing its symbol in the middle of a box in the table. The atomic number (Z) of the element is shown above the symbol, and the weighted-average atomic mass of the element is shown below its symbol.
- It is customary also to divide the elements into two broad categories metals and nonmetals.
- Two other highlighted categories in the periodic table are a special group of nonmetals known as the **noble gases** (pink), and a small group of elements, often called **metalloids** (green), that have some metallic and some nonmetallic properties.

The Periodic Table

- The sixth period is a long one of 32 members. To fit this period in a table that is held to a maximum width of 18 members, 15 members of the period are placed at the bottom of the periodic table.
- This series of 15 elements start with lanthanum (Z=57) and these elements are called the **lanthanides.**
- A15-member series is also extracted from the seventh period and placed at the bottom of the table. Because the elements in this series start with actinium (Z=89) they are called the **actinides**.
- **Main-group elements** are those in groups 1, 2, and 13 to 18.
- The elements in groups 3 to 12 are the **transition elements**, and because all of them are metals, they are also called the **transition metals**

The Mole

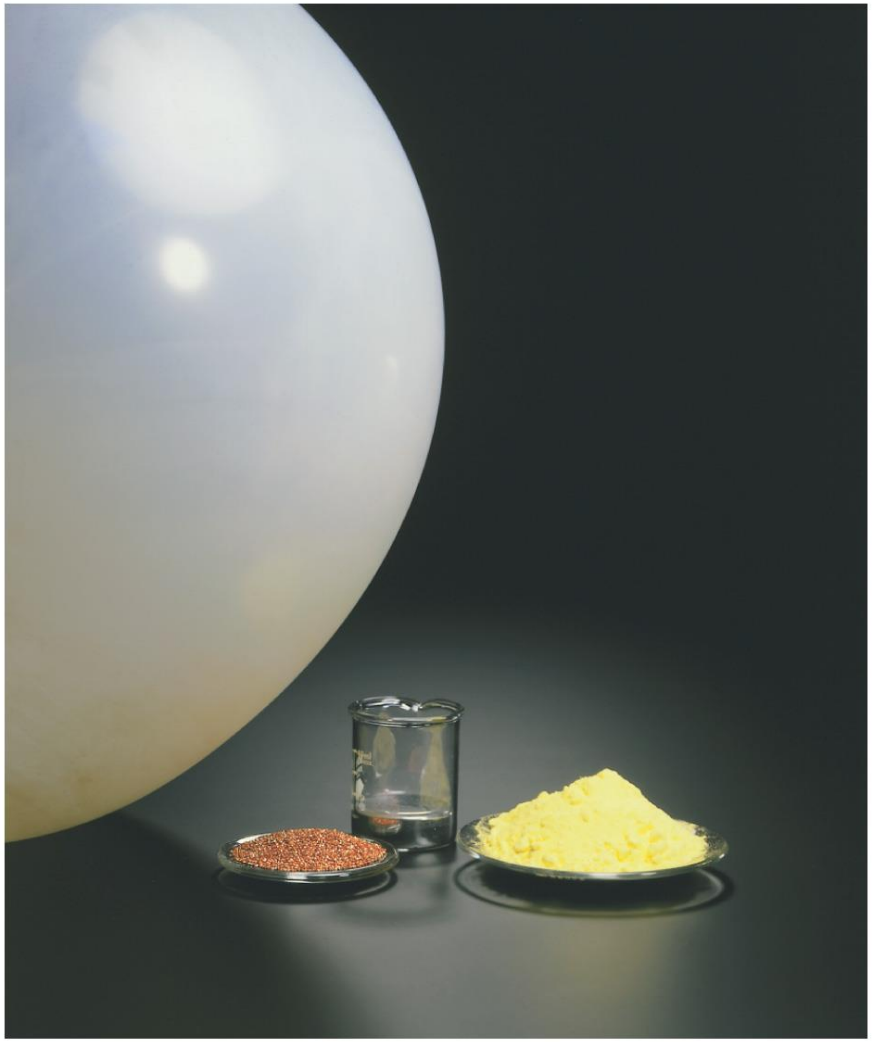
- Physically counting atoms is impossible.
- We must be able to relate measured mass to numbers of atoms.
  - buying nails by the pound or kilogram.
  - using atoms by the gram

Avogadro's number

- The mole is an amount of substance that contains the same number of elementary entities as there are carbon-12 atoms in *exactly* 12 g of carbon-12.

$$N_A = 6.02214199 \times 10^{23}\ \text{mol}^{-1}$$

The Mole



Molar Mass

- The molar mass, M, is the mass of one mole of a substance.

$$M\,(\text{g/mol } ^{12}\text{C}) = A\,(\text{g/atom } ^{12}\text{C}) \times N_A\,(\text{atoms } ^{12}\text{C /mol } ^{12}\text{C})$$

EXAMPLE 2-9

Combining Several Factors in a Calculation—Molar Mass, the Avogadro Constant, Percent Abundance. Potassium-40 is one of the few naturally occurring radioactive isotopes of elements of low atomic number. Its percent natural abundance among K isotopes is 0.012%. How many 40K atoms do you ingest by drinking one cup of whole milk containing 1.65 mg of K/mL?

Want atoms of ^{40}K, need atoms of K,

Want atoms of K, need moles of K,

Want moles of K, need total mass of K and *M*(K) (the molar mass).

EXAMPLE 2-9

Convert concentration of K (mg/mL K) into mass of K (g K)

$c_K(\text{mg/mL}) \times V\,(\text{mL}) \rightarrow m_K\,(\text{mg}) \times (1\text{g}/1000\text{mg}) \rightarrow m_K(\text{g})$

$n_K = (1.65\ \text{mg/mL K}) \times (225\ \text{mL}) \times (1\ \text{g}/1000\ \text{mg})$

$= 0.37l\ \text{g K}$

Convert mass of K(g K) into moles of K (mol K)

$m_K\,(\text{g}) \times 1/M_K\,(\text{mol/g}) \rightarrow n_K\,(\text{mol})$

$n_K = (0.371\ \text{g K}) \times (1\ \text{mol K}) / (39.10\ \text{g K})$

$= 9.49 \times 10^{-3}\ \text{mol K}$

EXAMPLE 2-9

Convert moles of K into atoms of ^{40}K

$n_K(\text{mol}) \times N_A \rightarrow$ atoms K $\times$ 0.012% $\rightarrow$ atoms ^{40}K

$$\text{atoms } ^{40}K = (9.49 \times 10^{-3} \text{ mol K}) \times (6.022 \times 10^{23} \text{ atoms K/mol K}) \times (1.2 \times 10^{-4}\ ^{40}K/K)$$

$$= 6.9 \times 10^{17}\ ^{40}K \text{ atoms}$$

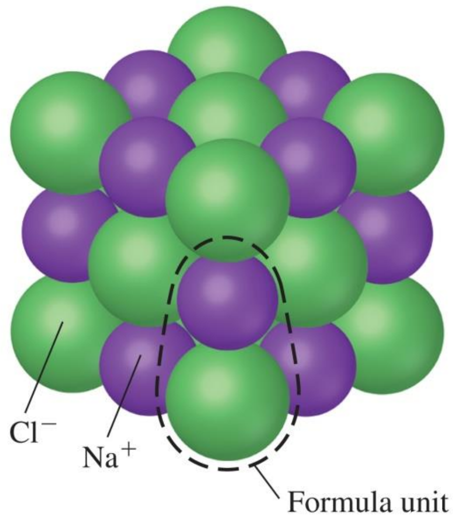
Note that the text shows two slightly different methods. There is often more than one correct way to solve a problem, but the strategy for the solution is often the same for any of the calculations.

Petrucci • Harwood • Herring • Madura

Ninth Edition

GENERAL CHEMISTRY

Principles and Modern Applications



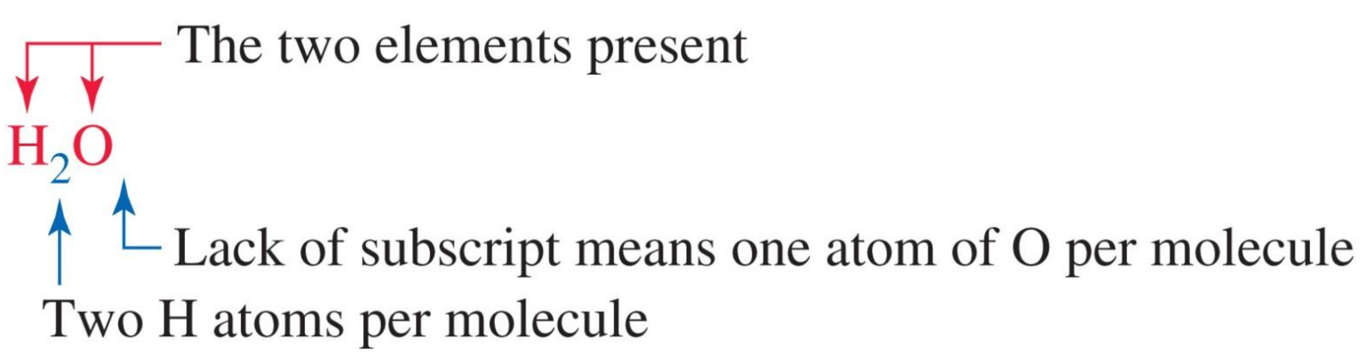
Chapter 3: Chemical Compounds

Contents

3-1 Types of Chemical Compounds and Their Formulas

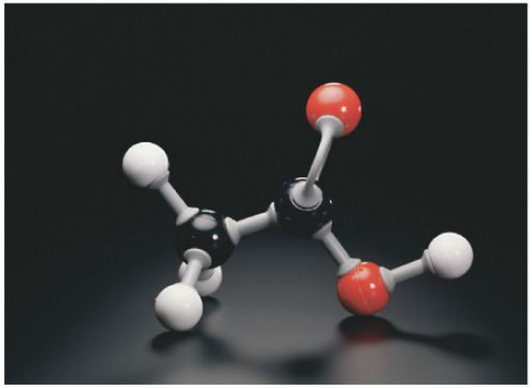
Molecular Compounds

- A **molecular compound** is made up of discrete units called **molecules**, which typically consist of a small number of *nonmetal* atoms held together by covalent bonds. Molecular compounds are represented by **chemical formulas**, symbolic representations that, at minimum, indicate the elements present the relative number of atoms of each element.
- In the formula for water, the constituent elements are denoted by their symbols. The relative numbers of atoms are indicated by *subscripts*. Where no subscript is written, the number 1 is understood.



Molecular compounds

- An **empirical formula** is the simplest formula for a compound; it shows the types of atoms present and their relative numbers.
- A **molecular formula** is based on an actual molecule of a compound. In some cases, the empirical and molecular formulas are identical, such as for formaldehyde. In other cases, the molecular formula is a multiple of the empirical formula.
- A **structural formula** shows the order in which atoms are bonded together in a molecule and by what types of bonds.

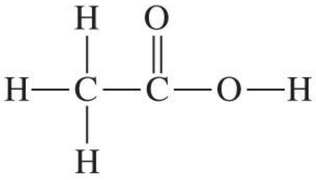


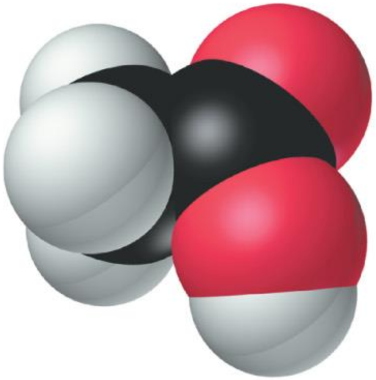
Molecular model:
("ball-and-stick")

Empirical formula: CH_2O

Molecular formula: $C_2H_4O_2$

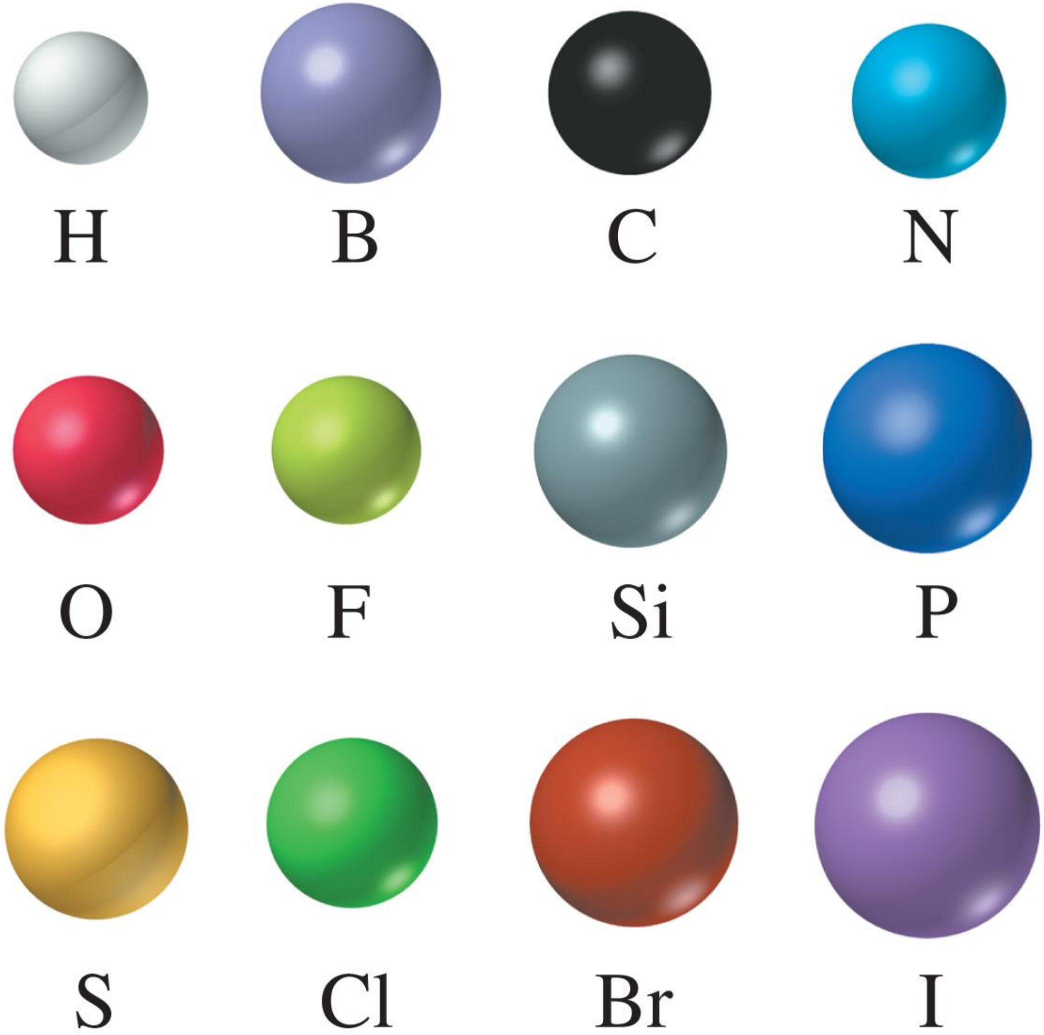
Structural formula:





Molecular model:
("space-filling")

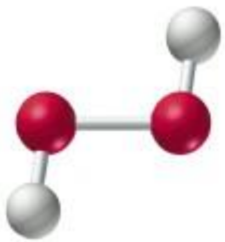
Standard Color Scheme



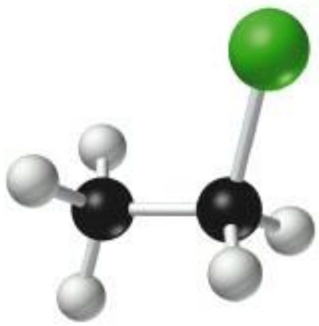
Some Organic and Inorganic Molecules

H_2O_2 CH_3CH_2Cl P_4O_{10}

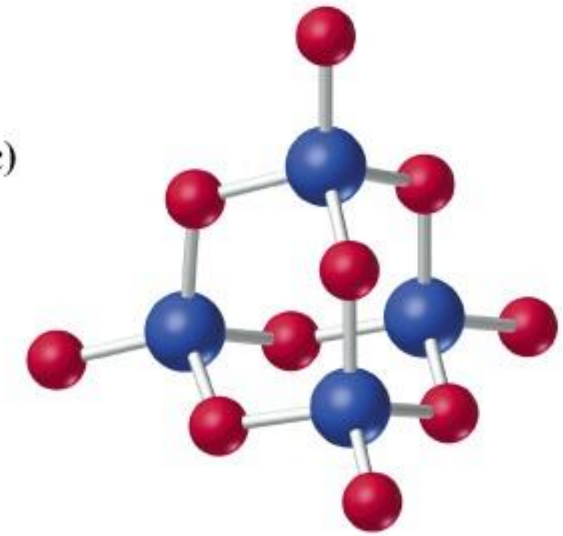
(a)



(b)

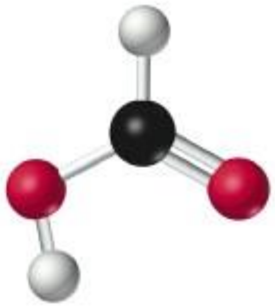


(c)



(d)

(e)



$CH_3CH(OH)CH_3$ HCO_2H

Ionic Compounds

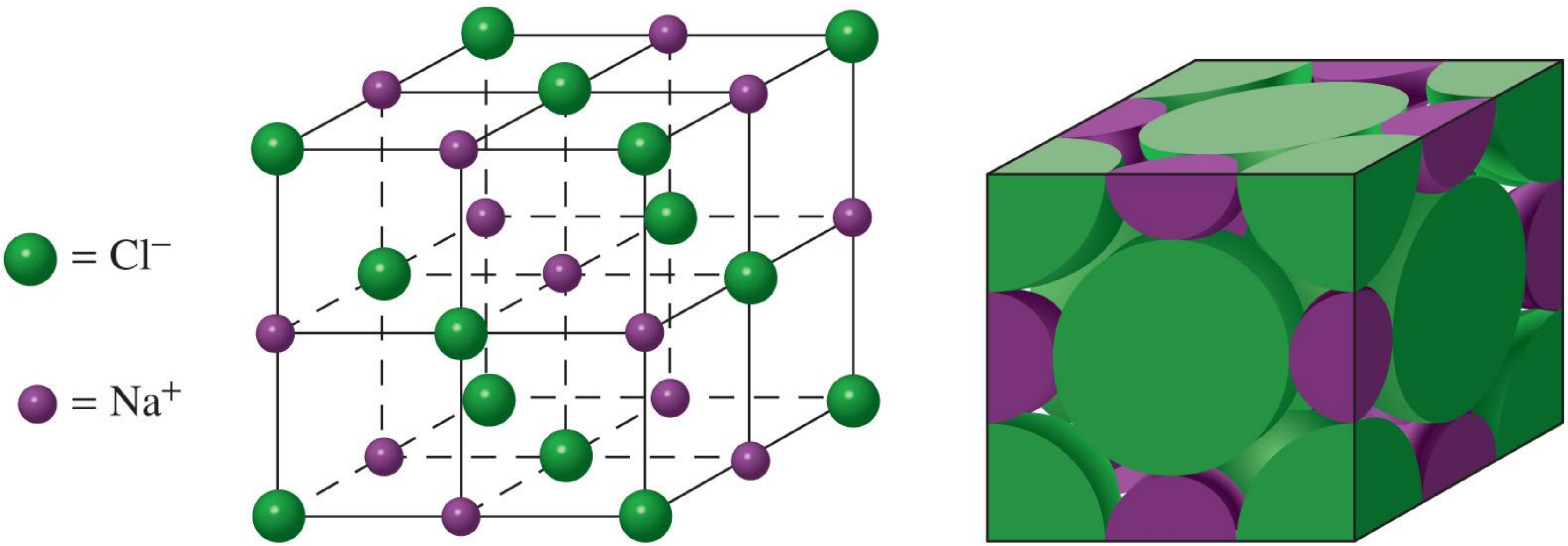
- ⌘ Atoms of almost all elements can gain *or* lose electrons to form charged species called **ions**.
- ⌘ Compounds composed of ions are known as **ionic compounds**.
- ⌘ An **ionic compound** is made up of positive and negative ions joined together by electrostatic forces of attraction.

  - ✓ Metals tend to lose electrons to form positively charged ions called **cations**.
  - ✓ Non-metals tend to gain electrons to form negatively charged ions called **anions**.

Sodium Chloride

An extended array of Na^+ and Cl^- ions

The simplest formula unit is NaCl



3-2 The Mole Concept and Chemical Calculations

- Formula mass
  - the mass of a formula unit in atomic mass units (u)
- Molecular mass
  - a formula mass of a *molecular compound*

Thus, for the molecular compound water, H_2O,

$$\begin{aligned} \text{molecular mass } H_2O &= 2(\text{atomic mass H}) + (\text{atomic mass O}) \\ &= 2(1.00794 \text{ u}) + 15.9994 \text{ u} \\ &= 18.0153 \text{ u} \end{aligned}$$

For the ionic compound magnesium chloride, $MgCl_2$,

$$\begin{aligned} \text{formula mass } MgCl_2 &= \text{atomic mass Mg} + 2(\text{atomic mass Cl}) \\ &= 24.3050 \text{ u} + 2(35.453 \text{ u}) \\ &= 95.211 \text{ u} \end{aligned}$$

EXAMPLE 3-2

Combining Several Factors in a Calculation Involving Molar Mass. The volatile liquid ethyl mercaptan, C_2H_5SH is one of the most odoriferous substances known. It is sometimes added to natural gas to make gas leaks detectable. How many C_2H_5SH molecules are contained in a 1.0 µL sample given the following information?

d= 0.84 g/mL C_2H_5SH=62.1 g/mol

EXAMPLE 7-3

Solution.

The strategy to follow can be laid out in a flow diagram.

$$\mu L \xrightarrow{10^{-6}\ L/\mu L} L \xrightarrow{10^{3}\ mL/L} mL \xrightarrow{0.84\ g/mL} g \xrightarrow{\frac{1\ mol}{62.1\ g}} mol \xrightarrow{6.02\ 10^{23}\ molec/mol} molecules$$

The factors in each conversion may be added above the arrows.

Don't worry if your conversion factors are upside down, fix them when you write the equations by making sure the units cancel properly.

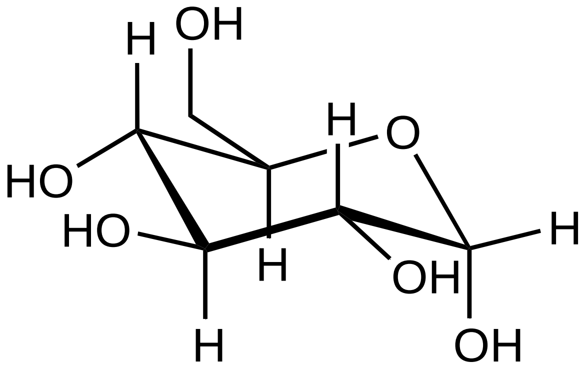
Using the strategy and the conversion factors, write the equation:

$$1\ \cancel{\mu L} \times 10^{-6}\ \cancel{L}/\cancel{\mu L} \times 10^{3}\ \cancel{mL}/\cancel{L} \times 0.84\ \cancel{g}/\cancel{mL} \times \frac{1\ \cancel{mol}}{62.1\ \cancel{g}} \times 6.02 \times 10^{23}\ molec/\cancel{mol}$$

Check the units cancel and *only then* calculate.

$$= 8.1 \times 10^{18}\ molecules$$

Molecular Mass



Glucose

Molecular formula $C_6H_{12}O_6$

Empirical formula CH_2O

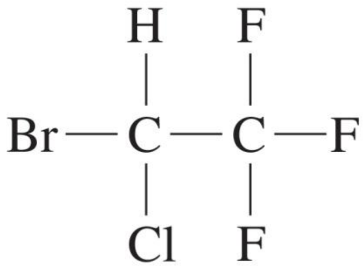
Molecular Mass: Use the naturally occurring mixture of isotopes,

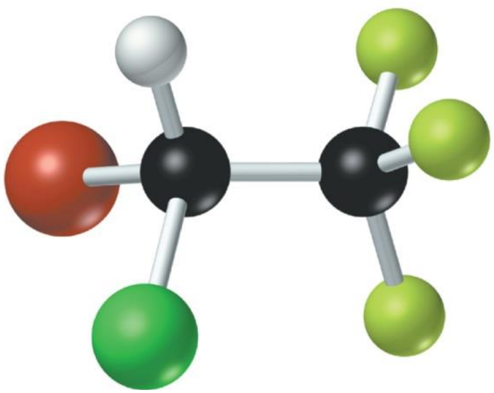
$$\mathbf{6} \times 12.01 \quad + \quad \mathbf{12} \times 1.01 \quad + \quad \mathbf{6} \times 16.00 = 180.18$$

Exact Mass: Use the most abundant isotopes,

$$\mathbf{6} \times 12.000000 \quad + \quad \mathbf{12} \times 1.007825 + \quad \mathbf{6} \times 15.994915$$
$$= 180.06339$$

3-3 Composition of Chemical Compounds





Halothane	$C_2HBrClF_3$
Mole ratio	$n_C/n_{halothane}$
Mass ratio	$m_C/m_{halothane}$

$$M(C_2HBrClF_3) = 2M_C + M_H + M_{Br} + M_{Cl} + 3M_F$$

$$= (2 \times 12.01) + 1.01 + 79.90 + 35.45 + (3 \times 19.00)$$

$$= 197.38 \text{ g/mol}$$

Calculating Percent Composition from a Chemical Formula

1. **Determine the molar mass of the compound.** This is the *denominator* in equation (3.1).
2. **Determine the contribution of the given element to the molar mass.** This product of the formula subscript and the molar mass of the element appears in the *numerator* of equation (3.1).
3. **Formulate the ratio of the mass of the given element to the mass of the compound as a whole.** This is the ratio of the numerator from step 2 to the denominator from step 1.
4. **Multiply this ratio by 100% to obtain the mass percent of the element.**

$$\text{mass \% element} = \frac{\begin{pmatrix}\text{number of} \\ \text{atoms of element} \\ \text{per formula unit}\end{pmatrix} \times \begin{pmatrix}\text{molar mass} \\ \text{of element}\end{pmatrix}}{\text{molar mass of compound}} \times 100\% \qquad \textbf{(3.1)}$$

The mass composition of a compound is the collection of mass percentages of the individual elements in the compound.

EXAMPLE 7-3

Calculating the Mass Percent Composition of a Compound

What is the mass percent composition of halothane, $C_2HBrClF_3$?

Calculate the molecular mass

$$M(C_2HBrClF_3) = 197.38 \text{ g/mol}$$

For one mole of compound, formulate the mass ratio and convert to percent:

$$\%C = \frac{\left(2 \text{ mol C} \times \left(\frac{12.01 \text{ g C}}{1 \text{ mol C}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 12.17\%$$

EXAMPLE 7-3

$$\%H = \frac{\left(1 \text{ mol H} \times \left(\frac{1.01 \text{ g H}}{1 \text{ mol H}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 0.51\% \text{ H}$$

$$\%Br = \frac{\left(1 \text{ mol Br} \times \left(\frac{79.90 \text{ g Br}}{1 \text{ mol Br}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 40.48\% \text{ Br}$$

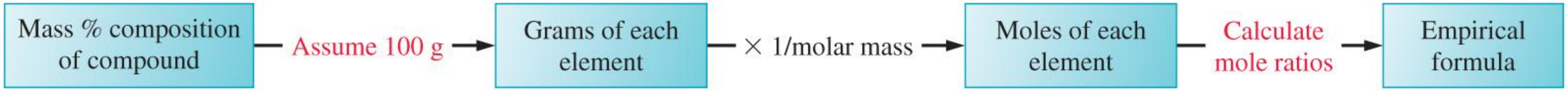
$$\%Cl = \frac{\left(1 \text{ mol C} \times \left(\frac{35.45 \text{ g Cl}}{1 \text{ mol Cl}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 17.96\% \text{ Cl}$$

$$\%F = \frac{\left(3 \text{ mol C} \times \left(\frac{19.00 \text{ g F}}{1 \text{ mol F}}\right)\right)}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 28.88\% \text{ F}$$

Establishing Formulas from Experimentally Determined Percent Composition

5 Step approach:

1. Choose an arbitrary sample size (100g).
2. Convert masses to amounts in moles.
3. Write a formula.
4. Convert formula to small whole numbers.
5. Multiply all subscripts by a small whole number to make the subscripts integral.



EXAMPLE 3-5

Determining the Empirical and Molecular Formulas of a Compound from Its Mass Percent Composition

Dibutyl succinate is an insect repellent used against household ants and roaches. Its composition is 62.58% C, 9.63% H and 27.79% O. Its experimentally determined molecular mass is 230 u. What are the empirical and molecular formulas of dibutyl succinate?

Step 1: Determine the mass of each element in a 100g sample.

C 62.58 g H 9.63 g O 27.79 g

EXAMPLE 3-5

Step 2: Convert masses to amounts in moles.

$$n_C = 62.58\ g\,C \times \frac{1\,mol\,C}{12.011\ g\,C} = 5.210\ mol\,C$$

$$n_H = 9.63\ g\,H \times \frac{1\,mol\,H}{1.008\ g\,H} = 9.55\ mol\,H$$

$$n_O = 27.79\ g\,O \times \frac{1\,mol\,O}{15.999\ g\,O} = 1.737\ mol\,O$$

Step 3: Write a tentative formula. $C_{5.21}H_{9.55}O_{1.74}$

Step 4: Convert to small whole numbers. $C_{2.99}H_{5.49}O$

EXAMPLE 3-5

Step 5: Convert to a small whole number ratio.

Multiply $\times$ 2 to get $C_{5.98}H_{10.98}O_2$

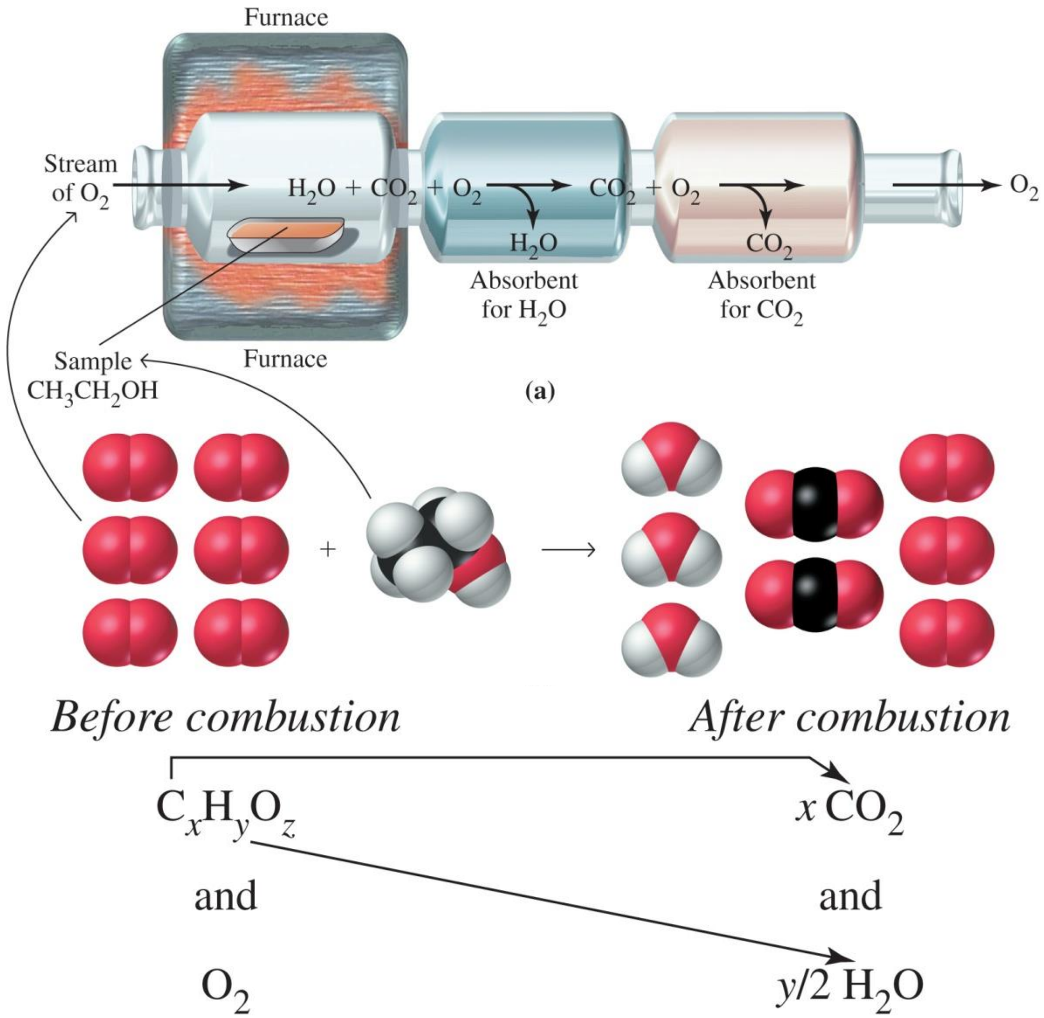
The empirical formula is $C_6H_{11}O_2$

Step 6: Determine the molecular formula.

Empirical formula mass is 115 u.
Molecular formula mass is 230 u.

The molecular formula is $C_{12}H_{22}O_4$

Combustion Analysis



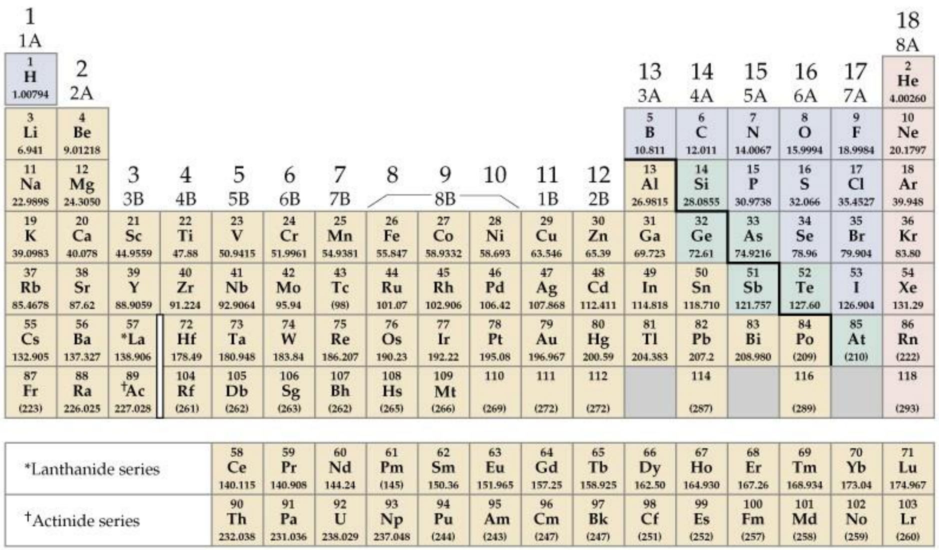
3-4 Oxidation States: A Useful Tool in Describing Chemical Compounds

Metals tend to lose electrons.

$Na \rightarrow Na^{+} + e^{-}$

Non-metals tend to gain electrons.

$Cl + e^{-} \rightarrow Cl^{-}$



Reducing agents

Oxidizing agents

We use the Oxidation State to keep track of the number of electrons that have been gained or lost by an element.

Rules for Oxidation States

1. The oxidation state (OS) of an individual atom in a free element is 0.

2. The total of the OS in all atoms in:
   i. Neutral species is 0.
   ii. Ionic species is equal to the charge on the ion.

3. In their compounds, the alkali metals and the alkaline earths have OS of +1 and +2 respectively.

4. In compounds the OS of fluorine is *always* –1

Rules for Oxidation States

5. In compounds, the OS of hydrogen is *usually* +1

6. In compounds, the OS of oxygen is *usually* –2.

7. In binary (two-element) compounds with metals:
    i. Halogens have OS of –1,
    ii. Group 16 have OS of –2 and
    iii. Group 15 have OS of –3.

EXAMPLE 3-7

Assigning Oxidation States What is the oxidation state of the underlined element in each of the following? a) P_4; b) Al_2O_3; c) MnO_4^-; d) NaH.

a) P_4 is an element. P OS = 0

b) Al_2O_3: O is –2. O_3 is –6. Since (+6)/2=(+3), Al OS = +3.

c) MnO_4^-: net OS = -1, O_4 is –8. Mn OS = +7.

d) NaH: net OS = 0, rule 3 beats rule 5, Na OS = +1 and H OS = -1.