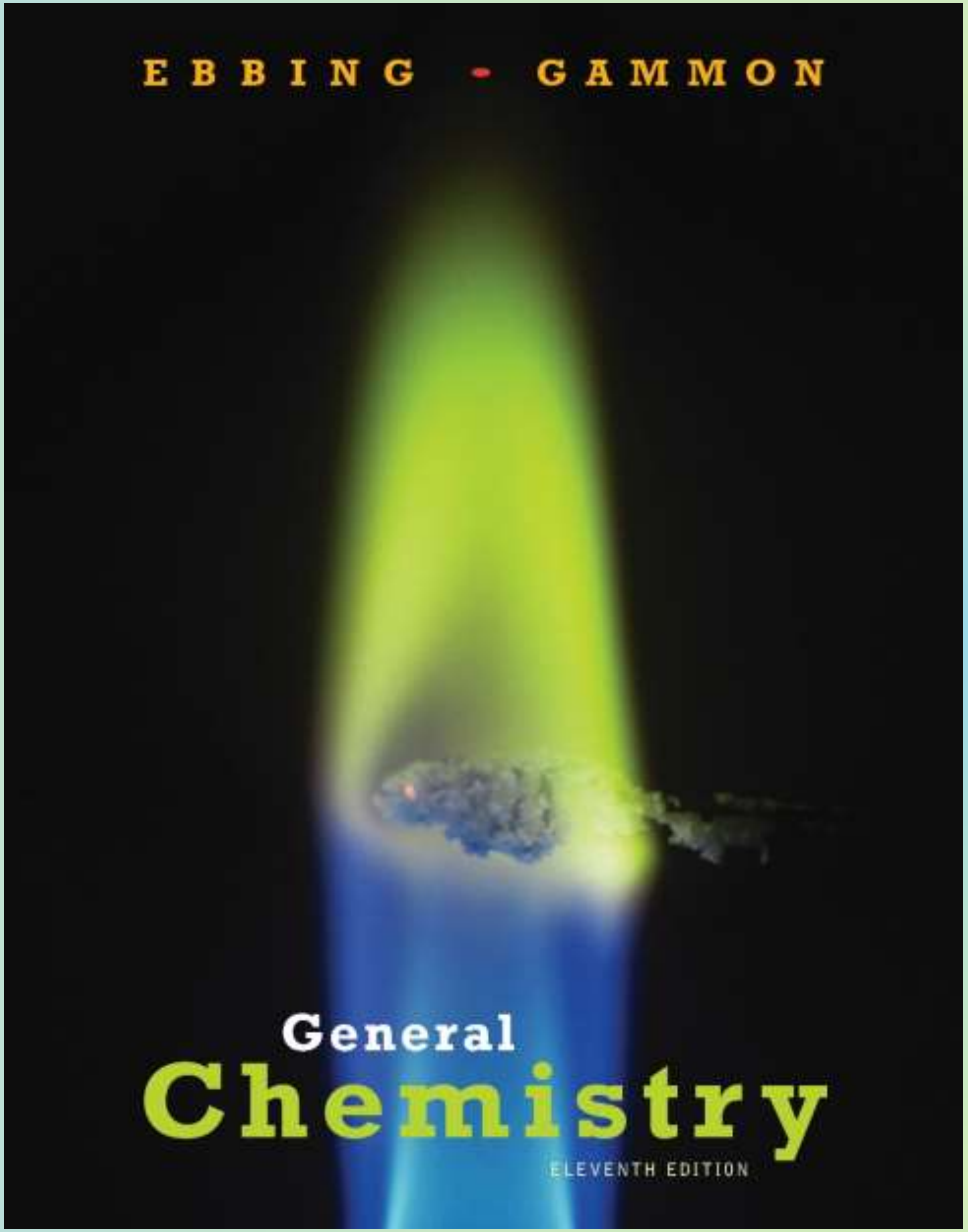
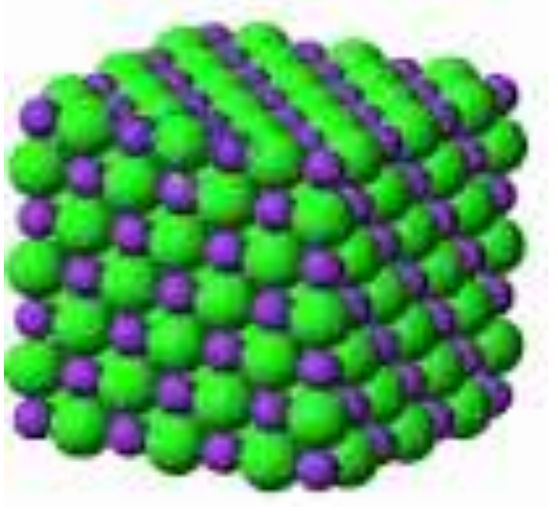


Calculations with Chemical Formulas and Equations

3.1 Molecular Weight and Formula Weight

molecular weight (MW) of a substance is: *the sum of the atomic weights of all the atoms in a molecule of the substance.*
Example: H_2O, is 18.0 amu
(2 x 1.0 amu +16.0 amu) =18 amu

formula weight (FW) of a substance is: *the sum of the atomic weights of all atoms in* ***a formula unit*** *of the compound,* whether molecular or not.
Example: NaCl, has a formula weight of 58.44 amu
(22.99 amu + 35.45 amu) = 58.44 amu



Main-Group Elements

Main-Group Elements

Transition Metals

1 **H** 1.00794	
Atomic number	Symbol
	Atomic mass

	1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 **H** 1.00794																	2 **He** 4.002602
2	3 **Li** 6.941	4 **Be** 9.012182											5 **B** 10.811	6 **C** 12.0107	7 **N** 14.0067	8 **O** 15.9994	9 **F** 18.9984032	10 **Ne** 20.1797
3	11 **Na** 22.98976928	12 **Mg** 24.3050											13 **Al** 26.9815386	14 **Si** 28.0855	15 **P** 30.973762	16 **S** 32.065	17 **Cl** 35.453	18 **Ar** 39.948
4	19 **K** 39.0983	20 **Ca** 40.078	21 **Sc** 44.955912	22 **Ti** 47.867	23 **V** 50.9415	24 **Cr** 51.9961	25 **Mn** 54.938045	26 **Fe** 55.845	27 **Co** 58.933195	28 **Ni** 58.6934	29 **Cu** 63.546	30 **Zn** 65.409	31 **Ga** 69.723	32 **Ge** 72.64	33 **As** 74.92160	34 **Se** 78.96	35 **Br** 79.904	36 **Kr** 83.798
5	37 **Rb** 85.4678	38 **Sr** 87.62	39 **Y** 88.90585	40 **Zr** 91.224	41 **Nb** 92.90638	42 **Mo** 95.94	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.90550	46 **Pd** 106.42	47 **Ag** 107.8682	48 **Cd** 112.411	49 **In** 114.818	50 **Sn** 118.710	51 **Sb** 121.760	52 **Te** 127.60	53 **I** 126.90447	54 **Xe** 131.293
6	55 **Cs** 132.9054519	56 **Ba** 137.327	71 **Lu** 174.967	72 **Hf** 178.49	73 **Ta** 180.94788	74 **W** 183.84	75 **Re** 186.207	76 **Os** 190.23	77 **Ir** 192.217	78 **Pt** 195.084	79 **Au** 196.966569	80 **Hg** 200.59	81 **Tl** 204.3833	82 **Pb** 207.2	83 **Bi** 208.98040	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
7	87 **Fr** (223)	88 **Ra** (226)	103 **Lr** (262)	104 **Rf** (261)	105 **Db** (262)	106 **Sg** (266)	107 **Bh** (264)	108 **Hs** (277)	109 **Mt** (268)	110 **Ds** (281)	111 **Rg** (272)	112 **Uub** (285)	113 **Uut** (284)	114 **Uuq** (289)	115 **Uup** (288)	116 **Uuh** (291)		118 **Uuo** (294)

Example 3.1 Calculating the Formula Weight from a Formula

Calculate the formula weight of each of the following to three significant figures, using a table of atomic weights (AW):

a. chloroform, $CHCl_3$ b. iron(III) sulfate, $Fe_2(SO_4)_3$.

$$
\begin{array}{llr}
1 \times \text{AM of C} = & & 12.0 \text{ amu} \\
1 \times \text{AM of H} = & & 1.0 \text{ amu} \\
3 \times \text{AM of Cl} = & 3 \times 35.45 \text{ amu} = & \underline{106.4 \text{ amu}} \\
\text{FM of } CHCl_3 = & & 119.4 \text{ amu}
\end{array}
$$

$$
\begin{array}{llr}
2 \times \text{AM of Fe} = & 2 \times 55.8 \text{ amu} = & 111.6 \text{ amu} \\
3 \times \text{AM of S} = & 3 \times 32.1 \text{ amu} = & 96.3 \text{ amu} \\
3 \times 4 \times \text{AM of O} = & 12 \times 16.00 \text{ amu} = & \underline{192.0 \text{ amu}} \\
\text{FM of } Fe_2(SO_4)_3 = & & 399.9 \text{ amu}
\end{array}
$$

3.2 The Mole Concept

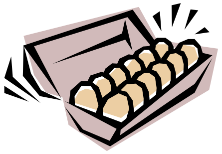
The Mole (mol): A unit to count numbers of particles

A mole (symbol mol) is defined as *the quantity of a given substance that contains as many molecules or formula units as the number of atoms in exactly 12 g of carbon-12*

Pair = 2

$1 \text{ mol} = N_A = 6.0221415 \times 10^{23}$ = Avogadro's number

Dozen = 12



1 mole of Na_2CO_3 contains 6.02×10^{23} Na_2CO_3 units

1 mole of Na_2CO_3 contains $2 \times 6.02 \times 10^{23}$ Na^+ ions

1 mole of Na_2CO_3 contains 6.02×10^{23} CO_3^{2-} ions

molar mass of a substance is *the mass of one mole of the substance.*

C has a molar mass of exactly 12 g/mol,

C_2H_5OH has a molar mass of exactly 46.1 g/mol

For any element

atomic mass (amu) = molar mass (grams)

➢ Mole Calculations

(Q) A chemist determines from the amounts of elements that 0.0654 mol ZnI_2 can form. How many grams of zinc iodide is this?
molar mass of ZnI_2 is 319 g/mol

Number of moles = mass(g) / molar mass

(Q)In a preparation rxn., 45.6 g of lead(II) chromate is obtained as a precipitate. How many moles of $PbCrO_4$ is this?
molar mass of $PbCrO_4$ = 323 g/mol

(Q) How many molecules are there in a 3.46-g sample of hydrogen chloride, HCl?

(Q) How many S atoms are there in 16.3 g of S?

Example 3.3 Calculating the Mass of an Atom or Molecule

a. What is the mass in grams of one chlorine atom, Cl?

b. What is the mass in grams of one HCl molecule?

(Q) How much, in grams, do 8.85×10^{24} atoms of zinc weigh?

A. 3.49×10^{49} g

B. 961 g

C. 4.45 g

D. 5.33×10^{47} g

E. 1.47 g

$$8.85 \times 10^{24}\,\cancel{\text{atoms}} \times \left(\frac{1\,\cancel{\text{mol}}}{6.022 \times 10^{23}\,\cancel{\text{atoms}}} \right) \times \left(\frac{65.41\text{ g Zn}}{1\,\cancel{\text{mol}}} \right)$$

= 961 g Zn

(Q) How many hydrogen atoms are present in 25.6 g of urea [$(NH_2)_2CO$]? molar mass of urea = 60.06 g/mol.

$$\text{grams of urea} \longrightarrow \text{moles of urea} \longrightarrow \text{moles of H} \longrightarrow \text{atoms of H}$$

$$25.6\ \cancel{\text{g }(NH_2)_2CO} \times \frac{1\ \cancel{\text{mol }(NH_2)_2CO}}{60.06\ \cancel{\text{g }(NH_2)_2CO}} \times \frac{4\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol }(NH_2)_2CO}} \times \frac{6.022 \times 10^{23}\ \text{H atoms}}{1\ \cancel{\text{mol H}}}$$

$= 1.03 \times 10^{24}$ H atoms

(Q) Calculate the number of moles of calcium in 2.53 moles of $Ca_3(PO_4)_2$

A. 2.53 mol Ca

B. 0.432 mol Ca

C. 3.00 mol Ca

D. 7.59 mol Ca

E. 0.843 mol Ca

2.53 moles of $Ca_3(PO_4)_2$ = ? mol Ca

3 mol Ca $\Leftrightarrow$ 1 mol $Ca_3(PO_4)_2$

$$2.53\,\text{mol}\,\cancel{Ca_3(PO_4)_2}\left(\frac{3\,\text{mol}\,Ca}{1\,\text{mol}\,\cancel{Ca_3(PO_4)_2}}\right)$$

= 7.59 mol Ca

(Q) A sample of sodium carbonate, Na_2CO_3, is found to contain 10.8 moles of sodium. How many moles of oxygen atoms (O) are present in the sample?

A. 10.8 mol O

B. 7.20 mol O

C. 5.40 mol O

D. 32.4 mol O

E. 16.2 mol O

10.8 moles of Na = ? mol O

2 mol Na ⇔ 3 mol O

$$10.8\ \cancel{\text{mol Na}} \left(\frac{3\ \text{mol O}}{2\ \cancel{\text{mol Na}}} \right)$$

= 16.2 mol O

(Q) How many g of iron are required to use up all of 25.6 g of oxygen atoms (O) to form Fe_2O_3?

A. 59.6 g

B. 29.8 g

C. 89.4 g

D. 134 g

E. 52.4 g

mass O → mol O → mol Fe → mass Fe

25.6 g O → ? g Fe

3 mol O ⇔ 2 mol Fe

$$25.6\ \cancel{\text{g O}} \times \left(\frac{1\ \cancel{\text{mol O}}}{16.0\ \cancel{\text{g O}}}\right) \times \left(\frac{2\ \cancel{\text{mol Fe}}}{3\ \cancel{\text{mol O}}}\right) \times \left(\frac{55.845\ \text{g Fe}}{1\ \cancel{\text{mol Fe}}}\right)$$

= 59.6 g Fe

(Q) Silver is often found in nature as the ore, argentite (Ag_2S). How many grams of pure silver can be obtained from a 836 g rock of argentite?

mass Ag_2S → mol Ag_2S → mol Ag → mass Ag

A. 7.75 g

B. 728 g

C. 364 g

D. 775 g

E. 418 g

836 g Ag_2S → ? g Ag

1 mol Ag_2S ⇔ 2 mol Ag

$$836\text{ g }\cancel{\text{Ag}_2\text{S}}\times\left(\frac{1\text{ mol }\cancel{\text{Ag}_2\text{S}}}{247.8\text{ g }\cancel{\text{Ag}_2\text{S}}}\right)\times\left(\frac{2\text{ }\cancel{\text{mol Ag}}}{1\text{ mol }\cancel{\text{Ag}_2\text{S}}}\right)\times\left(\frac{107.9\text{ g Ag}}{1\text{ }\cancel{\text{mol Ag}}}\right)$$

= 728 g Ag

➢ Percentage Composition

$$\%\ \text{by mass of element} = \frac{\text{mass of element}}{\text{mass of sample}} \times 100\%$$

Example: A sample of a liquid with a mass of 8.657 g was decomposed into its elements and gave 5.217 g of carbon, 0.9620 g of hydrogen, and 2.478 g of oxygen.
What is the percentage composition of this compound?

$$\left(\frac{\text{g C}}{\text{g total}}\right) \times 100\% = \frac{5.217\ \text{g C}}{8.657\ \text{g}} \times 100\% = 60.26\%\ \text{C}$$

$$\left(\frac{\text{g H}}{\text{g total}}\right) \times 100\% = \frac{0.9620\ \text{g H}}{8.657\ \text{g}} \times 100\% = 11.11\%\ \text{H}$$

$$\left(\frac{\text{g O}}{\text{g total}}\right) \times 100\% = \frac{2.478\ \text{g O}}{8.657\ \text{g}} \times 100\% = 28.62\%\ \text{O}$$

Sum of percentages: 100 %

(Q) A sample was analyzed and found to contain 0.1417 g nitrogen and 0.4045 g oxygen.
What is the percentage composition of this compound?

Total sample mass = 0.1417 g + 0.4045 g = 0.5462 g

% Composition of N

$$\left(\frac{\text{g N}}{\text{g total}}\right)\times 100\% = \left(\frac{0.1417\text{ g N}}{0.5462\text{ g}}\right)\times 100\% \quad \mathbf{= 25.94\%\ N}$$

% Composition of O

$$\left(\frac{\text{g O}}{\text{g total}}\right)\times 100\% = \left(\frac{0.4045\text{ g O}}{0.5462\text{ g}}\right)\times 100\% \quad \mathbf{= 74.06\%\ O}$$

(Q) a.Calculate the mass percentages of the elements in formaldehyde (CH_2O) molar mass = 30g/mol

$$\% \mathbf{C} = \frac{12.0\text{ g}}{30.0\text{ g}} \times 100\% = \mathbf{40.0\%}$$

$$\% \mathbf{H} = \frac{2 \times 1.01\text{ g}}{30.0\text{ g}} \times \mathbf{100\%} = \mathbf{6.73\%}$$

% **O** = 16/30 x100% = 53.3 %

$$\% \mathbf{O} = 100\% - (40.0\% + 6.73\%) = \mathbf{53.3\%}$$

b. How many grams of carbon are there in 83.5 g of CH_2O?

CH_2O is 40.0% C, so the mass of carbon in 83.5 g CH_2O is:
83.5 g X 0.400 = **33.4 g**

(Q) Calculate the mass percentages of the elements in H_3PO_4
molar mass = 97.99 g/mol

$$\%H = \frac{3(1.008\text{ g})\ H}{97.99\text{ g } H_3PO_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\text{ g } P}{97.99\text{ g } H_3PO_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\text{ g})\ O}{97.99\text{ g } H_3PO_4} \times 100\% = 65.31\%$$

➢Determining Empirical and Molecular Formulas

Empirical Formula

– Simplest ratio of atoms of each element in compound

– Obtained from experimental analysis of compound

Molecular Formula

– Exact composition of one molecule

– Exact whole number ratio of atoms of each element in molecule

glucose

Molecular formula $C_6H_{12}O_6$

Empirical formula CH_2O

➢ Three Ways to Calculate Empirical Formulas

1. **From Masses of Elements**

   e.g., 2.448 g sample of which 1.771 g is Fe and 0.677 g is O.

2. **From Percentage Composition**

   e.g., 43.64% P and 56.36% O

3. **From Combustion Data**

   - Given masses of combustion products

   e.g., The combustion of a 5.217 g sample of a compound of C, H, and O in pure oxygen gave 7.406 g CO_2 and 4.512 g of H_2O

1. Empirical Formula from Mass Data

When a 0.1156 g sample of a compound was analyzed, it was found to contain 0.04470 g of C, 0.01875 g of H, and 0.05215 g of N. Calculate the empirical formula of this compound.

Step 1: Calculate moles of each substance

$$0.04470\,\cancel{\text{g C}} \times \frac{1\,\text{mol C}}{12.011\,\cancel{\text{g C}}} = 3.722 \times 10^{-3}\ \text{mol C}$$

$$0.01875\,\cancel{\text{g H}} \times \frac{1\,\text{mol H}}{1.008\,\cancel{\text{g H}}} = 1.860 \times 10^{-2}\ \text{mol H}$$

$$0.05215\,\cancel{\text{g N}} \times \frac{1\,\text{mol N}}{14.0067\,\cancel{\text{g N}}} = 3.723 \times 10^{-3}\ \text{mol N}$$

Step 2: Select the smallest number of moles

- Smallest is 3.722×10^{-3} mole

Mole ratio Integer ratio

- $C = \dfrac{3.722 \times 10^{-3} \text{ mol C}}{3.722 \times 10^{-3} \text{ mol C}} = 1.000 \quad = 1$

- $H = \dfrac{1.860 \times 10^{-2} \text{ mol H}}{3.722 \times 10^{-3} \text{ mol C}} = 4.997 \quad = 5$

- $N = \dfrac{3.723 \times 10^{-3} \text{ mol N}}{3.722 \times 10^{-3} \text{ mol C}} = 1.000 \quad = 1$

Step 3: Divide all number of moles by the smallest one

Empirical formula = CH_5N

2. Empirical Formula from Percentage Composition

Calculate the empirical formula of a compound whose percentage composition data is 43.64% P and 56.36% O. If the molar mass is determined to be 283.9 g/mol, what is the molecular formula?

Step 1: Assume 100 g of compound

- 43.64 g P — 1 mol P = 30.97 g
- 56.36 g O — 1 mol O = 16.00 g

$$43.64\ \cancel{g\,P} \times \frac{1\ mol\ P}{30.97\ \cancel{g\,P}} = 1.409\ mol\ P$$

$$56.36\ \cancel{g\,O} \times \frac{1\ mol\ O}{16.00\ \cancel{g\,O}} = 3.523\ mol\ O$$

Step 2: Divide by smallest number of moles

$$\frac{1.409\ \text{mol P}}{1.409\ \text{mol P}} = 1.000$$

$$\frac{3.523\ \text{mol O}}{1.409\ \text{mol P}} = 2.500$$

Step 3: Multiple to get integers

$$1.000 \times 2 = 2$$
$$2.500 \times 2 = 5$$

Empirical formula = P_2O_5

(Q) Ascorbic acid (vitamin C) is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

Assume you have 100 g.

$$n_C = 40.92\ \cancel{g\,C} \times \frac{1\ \text{mol C}}{12.01\ \cancel{g\,C}} = 3.407\ \text{mol C}$$

$$n_H = 4.58\ \cancel{g\,H} \times \frac{1\ \text{mol H}}{1.008\ \cancel{g\,H}} = 4.54\ \text{mol H}$$

→formula $C_{3.407}H_{4.54}O_{3.406}$

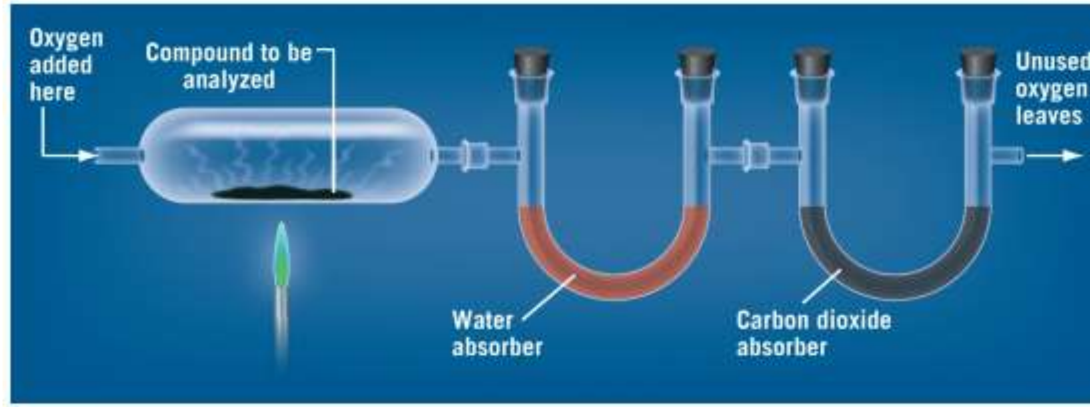
$$n_O = 54.50\ \cancel{g\,O} \times \frac{1\ \text{mol O}}{16.00\ \cancel{g\,O}} = 3.406\ \text{mol O}$$

$$C: \frac{3.407}{3.406} \approx 1 \qquad H: \frac{4.54}{3.406} = 1.33 \qquad O: \frac{3.406}{3.406} = 1$$

→formula $C_1H_{1.33}O_1$ X 3 → formula $C_3H_4O_3$

3. Empirical Formulas from Indirect Analysis: (Combustion analysis)

Classic



Combustion Analysis

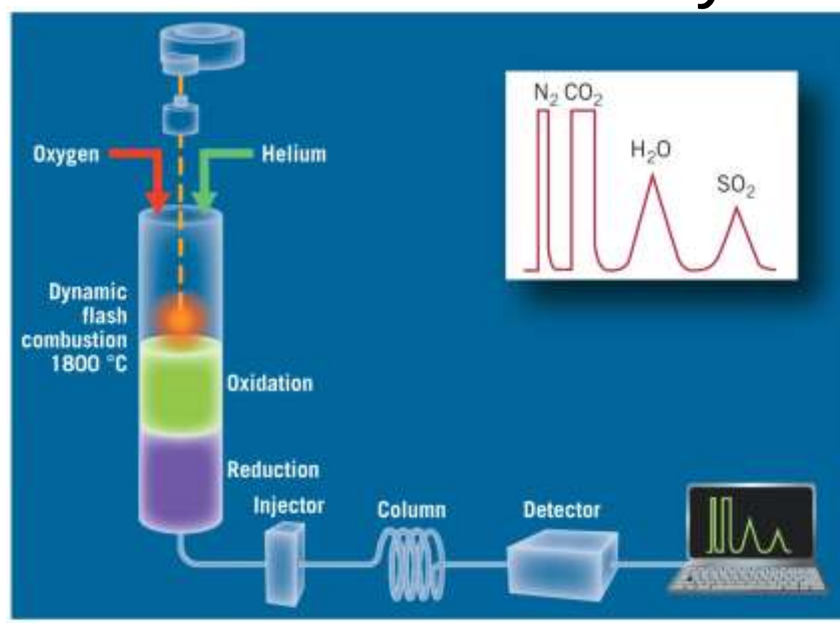
Compounds containing carbon, hydrogen, and oxygen, can be burned completely in pure oxygen gas.

Only carbon dioxide and water are produced

e.g., Combustion of methanol (CH_3OH)

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

Modern CHN analysis



- Carbon dioxide and water are separated and weighed separately
  - All C ends up as CO_2
  - All H ends up as H_2O
  - Mass of C can be derived from amount of CO_2
    - mass $CO_2 \rightarrow$ mol $CO_2 \rightarrow$ mol C $\rightarrow$ mass C
  - Mass of H can be derived from amount of H_2O
    - mass $H_2O \rightarrow$ mol $H_2O \rightarrow$ mol H $\rightarrow$ mass H
  - **Mass of oxygen is obtained by difference**
    - **mass O = mass sample – (mass C + mass H)**

(Q) The combustion of a 5.217 g sample of a compound of C, H, and O in pure oxygen gave 7.406 g CO_2 and 4.512 g of H_2O. Calculate the empirical formula of the compound.

1. Calculate mass of C from mass of CO_2.

mass $CO_2 \rightarrow$ mole $CO_2 \rightarrow$ mole C $\rightarrow$ mass C

$$7.406\,g\,CO_2\left(\frac{1\ mol\,CO_2}{44.01\,g\,CO_2}\right)\left(\frac{1\,mol\,C}{1\,mol\,CO_2}\right)\left(\frac{12.011\,g\,C}{1\ mol\,C}\right) \quad \mathbf{= 2.021\,g\,C}$$

2. Calculate mass of H from mass of H_2O.

mass $H_2O \rightarrow$ mol $H_2O \rightarrow$ mol H $\rightarrow$ mass H

$$4.512\,g\,H_2O\left(\frac{1\,mol\,H_2O}{18.015\,g\,H_2O}\right)\left(\frac{2\,mol\,H}{1\,mol\,H_2O}\right)\left(\frac{1.008\,g\,H}{1\,mol\,H}\right) \quad \mathbf{= 0.5049\,g\,H}$$

3. Calculate mass of O from difference.

5.217 g sample – 2.021 g C – 0.5049 g H **= 2.691 g O**

4. Calculate mol of each element

$$\text{mol C} = \frac{\text{g C}}{\text{MM C}} = \frac{2.021\text{ g}}{12.011\text{ g/mol}}$$ = 0.1683 mol C

$$\text{mol H} = \frac{\text{g H}}{\text{MM H}} = \frac{0.5049\text{ g}}{1.008\text{ g/mol}}$$ = 0.5009 mol H

$$\text{mol O} = \frac{\text{g O}}{\text{MM O}} = \frac{2.691\text{ g}}{15.999\text{ g/mol}}$$ = 0.1682 mol O

- Preliminary empirical formula

$C_{0.1683}H_{0.5009}O_{0.1682}$

5. Calculate mol ratio of each element

$$C_{\frac{0.1683}{0.1682}}H_{\frac{0.5009}{0.1682}}O_{\frac{0.1682}{0.1682}} = C_{1.00}H_{2.97}O_{1.00}$$

Empirical Formula = CH_3O

(Q) The combustion of a 13.660 g sample of a compound of C, H, and S in pure oxygen gave 19.352 g CO_2 and 11.882 g of H_2O. Calculate the empirical formula of the compound.

A. $C_4H_{12}S$
B. CH_3S
C. C_2H_6S
D. $C_2H_6S_3$
E. CH_3S_2

(1) mass CO_2 → mole CO_2 → mole C → mass C
(2) mass H_2O → mole H_2O → mole H → mass H
(3) Calculate mass of S from difference

$$19.352\ \text{g CO}_2\left(\frac{1\ \text{mol CO}_2}{44.01\ \text{g CO}_2}\right)\left(\frac{1\ \text{mol C}}{1\ \text{mol CO}_2}\right)\left(\frac{12.011\ \text{g C}}{1\ \text{mol C}}\right) = 5.281\ \text{g C}$$

$$11.882\ \text{g H}_2\text{O}\left(\frac{1\ \text{mol H}_2\text{O}}{18.015\ \text{g H}_2\text{O}}\right)\left(\frac{2\ \text{mol H}}{1\ \text{mol H}_2\text{O}}\right)\left(\frac{1.008\ \text{g H}}{1\ \text{mol H}}\right) = 1.330\ \text{g H}$$

13.66 g sample – 5.281 g C – 1.330 g H = 7.049 g S

$$\text{mol C} = \frac{\text{g C}}{\text{MM C}} = \frac{5.281\ \cancel{\text{g}}}{12.011\ \cancel{\text{g}}/\text{mol}} = 0.4497 \text{ mol C}$$

$$\text{mol H} = \frac{\text{g H}}{\text{MM H}} = \frac{1.330\ \cancel{\text{g}}}{1.008\ \cancel{\text{g}}/\text{mol}} = 1.319 \text{ mol H}$$

$$\text{mol S} = \frac{\text{g S}}{\text{MM S}} = \frac{7.049\ \cancel{\text{g}}}{32.065\ \cancel{\text{g}}/\text{mol}} = 0.2198 \text{ mol S}$$

- Preliminary empirical formula
  - $C_{0.4497}H_{1.319}S_{0.2198}$

$$C_{\frac{0.4497}{0.2198}}H_{\frac{1.319}{0.2198}}O_{\frac{0.2198}{0.2198}} = C_{2.03}H_{6.00}S_{1.00}$$

Empirical Formula = C_2H_6S

- Determining Molecular Formula from empirical formula

-In some cases molecular and empirical formulas are the same

-When they are different, the subscripts of molecular formula are integer multiples of those in empirical formula

- If empirical formula is A_xB_y
- Molecular formula will be $A_{(n\times x)}B_{(n\times y)}$

(Q)The empirical formula of hydrazine is NH_2, and its molecular mass is 32.0. What is its molecular formula?

Atomic masses: N = 14.007; H = 1.008; O = 15.999

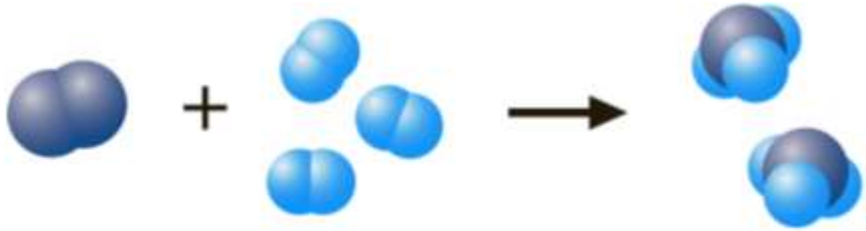
Molar mass of NH_2 = (1 × 14.01) g + (2 × 1.008) g = 16.017 g

n = (32.0/16.02) = 2

(NH_2) X 2 = N_2H_4

Stoichiometry:Quantitative Relations in Chemical Reactions

Molar Interpretation of a Chemical Equation



$$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$$

N_2	+	$3H_2$	$\longrightarrow$	$2NH_3$	
1 molecule N_2	+	3 molecules H_2	$\longrightarrow$	2 molecules NH_3	(molecular interpretation)
1 mol N_2	+	3 mol H_2	$\longrightarrow$	2 mol NH_3	(molar interpretation)
28.0 g N_2	+	3×2.02 g H_2	$\longrightarrow$	2×17.0 g NH_3	(mass interpretation)

3.7 Amounts of Substances in a Chemical Reaction

Example 3.13

Relating the Quantity of Reactant to Quantity of Product

In the following reaction:

$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$

How many grams of Fe(s) can be produced from 1.00 kg Fe_2O_3?

Molar masses are: Fe = 55.8 g/mol and Fe_2O_3 = 160 g/mol

Solution The calculation is as follows:

$$1.00 \times 10^3\ \cancel{\text{g Fe}_2\text{O}_3} \times \frac{1\ \cancel{\text{mol Fe}_2\text{O}_3}}{160\ \cancel{\text{g Fe}_2\text{O}_3}} \times \frac{2\ \cancel{\text{mol Fe}}}{1\ \cancel{\text{mol Fe}_2\text{O}_3}} \times \frac{55.8\ \text{g Fe}}{1\ \cancel{\text{mol Fe}}} = \mathbf{698\ g\ Fe}$$

Example 3.14

Relating the Quantities of Two Reactants (or Two Products)

In the following reaction:

$4HCl(aq) + MnO_2(s) \rightarrow 2H_2O(l) + MnCl_2(aq) + Cl_2(g)$

How many grams of HCl react with 5.00 g of MnO_2, according to this equation?

$$5.00\ \cancel{g\ MnO_2} \times \frac{1\ \cancel{mol\ MnO_2}}{86.9\ \cancel{g\ MnO_2}} \times \frac{4\ \cancel{mol\ HCl}}{1\ \cancel{mol\ MnO_2}} \times \frac{36.5\ g\ HCl}{1\ \cancel{mol\ HCl}} = \mathbf{8.40\ g\ HCl}$$

Exercise 3.16 oxygen can be prepared by heating mercury(II) oxide, HgO. Mercury metal is the other product. If 6.47 g of oxygen is collected, how many grams of mercury metal are also produced? $2HgO \rightarrow 2Hg + O_2$

$$6.47\ g\ O_2 \times \frac{1\ mol\ O_2}{32.00\ g\ O_2} \times \frac{2\ mol\ Hg}{1\ mol\ O_2} \times \frac{200.59\ g\ Hg}{1\ mol\ Hg} = 81.\underline{1}1 = 81.1\ g\ Hg$$

How many grams of Al_2O_3 are produced when 41.5 g Al react?

$$2Al(s) + Fe_2O_3(s) \rightarrow Al_2O_3(s) + 2Fe(l)$$

A. 78.4 g

B. 157 g

C. 314 g

D. 22.0 g

E. 11.0 g

$$41.5\ \cancel{\text{g Al}}\left(\frac{1\ \cancel{\text{mol Al}}}{26.98\ \cancel{\text{g Al}}}\right)\left(\frac{1\ \cancel{\text{mol Al}_2\text{O}_3}}{2\ \cancel{\text{mol Al}}}\right)\left(\frac{101.96\ \text{g Al}_2\text{O}_3}{1\ \cancel{\text{mol Al}_2\text{O}_3}}\right)$$

$$= 78.4\ \text{g Al}_2\text{O}_3$$

How many grams of sodium dichromate are required to produce 24.7 g iron(III) chloride from the following reaction?

$$14HCl + Na_2Cr_2O_7 + 6FeCl_2 \rightarrow 2CrCl_3 + 7H_2O + 6FeCl_3 + 2NaCl$$

A. 6.64 g $Na_2Cr_2O_7$

B. 0.152 g $Na_2Cr_2O_7$

C. 8.51 g $Na_2Cr_2O_7$

D. 39.9 g $Na_2Cr_2O_7$

E. 8.04 g $Na_2Cr_2O_7$

$$24.7\ \cancel{\text{g } FeCl_3} \times \left(\frac{1\ \cancel{\text{mol } FeCl_3}}{162.2\ \cancel{\text{g } FeCl_3}}\right) \times \left(\frac{1\ \cancel{\text{mol } Na_2Cr_2O_7}}{6\ \cancel{\text{mol } FeCl_3}}\right) \times \left(\frac{262.0\ \text{g } Na_2Cr_2O_7}{1\ \cancel{\text{mol } Na_2Cr_2O_7}}\right)$$

$= 6.64$ g $Na_2Cr_2O_7$

3.8 Limiting Reactant; Theoretical and Percentage Yields

Example 3.15 Calculating with a Limiting Reactant (Involving Moles)
Zinc metal reacts with hydrochloric acid by the following reaction:
$Zn(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$
If 0.30 mol Zn is added to a solution containing 0.52 mol HCl, how many moles of H_2 are produced?

3.91 Potassium superoxide, KO_2, is used in rebreathing gas masks to generate oxygen.
$4KO_2(s) + 2H_2O(l) \rightarrow 4KOH(s) + 3O_2(g)$
If a reaction vessel contains 0.25 mol KO_2 and 0.15 mol H_2O, what is the limiting reactant? How many moles of oxygen can be produced?

Calculating with a Limiting Reactant (Involving Masses)

3.96 Hydrogen cyanide, HCN, is prepared from ammonia, air, and natural gas (CH_4) by the following process:

$2NH_3(g) + 3O_2(g) + 2CH_4(g) \rightarrow 2HCN(g) + 6H_2O(g)$

If a reaction vessel contains 11.5 g NH_3, 12.0 g O_2, and 10.5 g CH_4, what is the maximum mass in grams of hydrogen cyanide that could be made, assuming the reaction goes to completion as written?

➢ Theoretical yield and percentage yield

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

3.97 Aspirin (acetylsalicylic acid) is prepared by heating salicylic acid, $C_7H_6O_3$, with acetic anhydride, $C_4H_6O_3$. The other product is acetic acid, $C_2H_4O_2$.

$C_7H_6O_3 + C_4H_6O_3 \rightarrow C_9H_8O_4 + C_2H_4O_2$

What is the theoretical yield (in grams) of aspirin, $C_9H_8O_4$, when 2.00 g of salicylic acid is heated with 4.00 g of acetic anhydride? If the actual yield of aspirin is 1.86 g, what is the percentage yield?

(Q) When 6.40 g of CH_3OH was mixed with 10.2 g of O_2 and ignited, 6.12 g of CO_2 was obtained. What was the percentage yield of CO_2?

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

MM(g/mol) (32.04) (32.00) (44.01) (18.02)

A. 6.12%

B. 8.79%

C. 100%

D. 142%

E. 69.6%

$$6.40\text{ g }CH_3OH \times \frac{1\text{ mol }CH_3OH}{32.04\text{ g }CH_3OH} \times \frac{3\text{ mol }CO_2}{2\text{ mol }CH_3OH} \times \frac{32.00\text{ g }O_2}{1\text{ mol }O_2}$$

$= 9.59$ g O_2 needed; CH_3OH limiting

$$6.40\text{ g }CH_3OH \times \frac{1\text{ mol }CH_3OH}{32.04\text{ g }CH_3OH} \times \frac{2\text{ mol }CO_2}{2\text{ mol }CH_3OH} \times \frac{44.01\text{ g }CO_2}{1\text{ mol }CO_2}$$

$= 8.79$ g CO_2 in theory

$$\frac{6.12\text{ g }CO_2\text{ actual}}{8.79\text{ g }CO_2\text{ theory}} \text{´}\ 100\ \% = 69.6\%$$