Chapter 6
Chemical Composition

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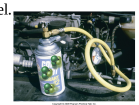
Chem 118
Introductory Chemistry

Map: Introductory Chemistry (Tro) https://chem.libretexts.org/@go/page/45050 (accessed Mar 25, 2022).

Why Is Knowledge of Composition Important?

- Everything in nature is either chemically or physically combined with other substances.
- To know the amount of a material in a sample, you need to know what fraction of the sample it is.
- Some Applications:
  - ✓ The amount of sodium in sodium chloride for diet.
  - ✓ The amount of iron in iron ore for steel production.
  - ✓ The amount of hydrogen in water for hydrogen fuel.
  - ✓ The amount of chlorine in freon to estimate ozone depletion.



The Mole

Counting Nails by the Pound

- I want to buy a certain number of nails for a project, but the hardware store sells nails by the pound.
- How do I know how many nails I am buying when I buy a pound of nails?
- Analogy:
  - ✓How many atoms in a given mass of an element?

Counting Nails by the Pound, Continued

A hardware store customer buys 2.60 pounds of nails. A dozen nails has a mass of 0.150 pounds. How many nails did the customer buy?

1 dozen nails = 0.150 lbs.

12 nails = 1 dozen nails

Solution map:

$$\text{lb nails} \xrightarrow{\frac{1\text{ doz nails}}{0.150\text{ lb nails}}} \text{doz nails} \xrightarrow{\frac{12\text{ nails}}{1\text{ doz nails}}} \text{number of nails}$$

Counting Nails by the Pound, Continued

$$2.60\,\cancel{\text{lbs.}} \times \frac{1\,\text{doz.}\,\cancel{\text{nails}}}{0.150\,\cancel{\text{lbs.}}} \times \frac{12\text{ nails}}{1\,\cancel{\text{doz.}}} = 208\text{ nails}$$

- The customer bought 2.60 lbs of nails and received 208 nails. He counted the nails by weighing them!

Counting Nails by the Pound, Continued

- What if he bought a different size nail?
  - ✓Would the mass of a dozen be 0.150 lbs?
  - ✓Would there still be 12 nails in a dozen?
  - ✓Would there be 208 nails in 2.60 lbs?
  - ✓How would this effect the conversion factors?

Counting Atoms by Moles

- If we can find the mass of a particular number of atoms, we can use this information to convert the mass of an element sample to the number of atoms in the sample.
- The number of atoms we will use is 6.022×10^{23} and we call this a **mole**.
  - ✓1 mole = 6.022×10^{23} things.
    - ➤Like 1 dozen = 12 things.
  - ✓Avogadro's number.

$$\frac{6.022 \times 10^{23}\text{ atoms}}{1\text{ mole}} \qquad \frac{1\text{ mole}}{6.022 \times 10^{23}\text{ atoms}}$$

Chemical Packages—Moles

- Mole = Number of things equal to the number of atoms in 12 g of C-12.
  - ✓1 atom of C-12 weighs exactly 12 amu.
  - ✓1 mole of C-12 weighs exactly 12 g.
- In 12 g of C-12 there are 6.022×10^{23} C-12 atoms.

Example 6.1—A Silver Ring Contains 1.1 x 10^{22} Silver Atoms. How Many Moles of Silver Are in the Ring?

Given: **Find:**	1.1×10^{22} atoms Ag moles Ag
Solution Map: **Relationships:**	atoms Ag $\xrightarrow{\frac{1\text{ mol}}{6.022 \times 10^{23}\text{ atoms}}}$ mol Ag 1 mol = 6.022×10^{23} atoms
Solution:	$1.1 \times 10^{22}\ \cancel{\text{atoms}}\text{ Ag} \times \frac{1\text{ mol}}{6.022 \times 10^{23}\ \cancel{\text{atoms}}}$ $= 1.8266 \times 10^{-2}\text{ mol Ag} = 1.8 \times 10^{-2}\text{ mol Ag}$
Check:	Since the number of atoms given is less than Avogadro's number, the answer makes sense.

Practice—Calculate the Number of Atoms in 2.45 Mol of Copper, Continued.

Given: **Find:**	2.45 mol Cu atoms Cu
Solution Map: **Relationships:**	mol Cu $\xrightarrow{\frac{6.022 \times 10^{23}\text{ atoms}}{1\text{ mol}}}$ atoms Cu 1 mol = 6.022×10^{23} atoms
Solution:	$2.45\ \cancel{\text{mol}}\text{ Cu} \times \frac{6.022 \times 10^{23}\text{ atoms}}{1\ \cancel{\text{mol}}}$ $= 1.48 \times 10^{24}\text{ atoms Cu}$
Check:	Since atoms are small, the large number of atoms makes sense.

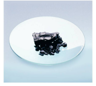
Relationship Between Moles and Mass

- The mass of one mole of atoms is called the **molar mass**.
- The molar mass of an element, in grams, is numerically equal to the element's atomic mass, in amu.
- The lighter the atom, the less a mole weighs.
- The lighter the atom, the more atoms there are in 1 g.

Mole and Mass Relationships

Substance	*Pieces in 1 mole*	*Weight of 1 mole*
Hydrogen	6.022×10^{23} atoms	1.008 g
Carbon	6.022×10^{23} atoms	12.01 g
Oxygen	6.022×10^{23} atoms	16.00 g
Sulfur	6.022×10^{23} atoms	32.06 g
Calcium	6.022×10^{23} atoms	40.08 g
Chlorine	6.022×10^{23} atoms	35.45 g
Copper	6.022×10^{23} atoms	63.55 g

1 mole sulfur 32.06 g



1 mole carbon 12.01 g

Example 6.2—Calculate the Moles of Sulfur in 57.8 G of Sulfur.

Given: **Find:**	57.8 g S mol S
Solution Map: **Relationships:**	g S $\xrightarrow{\frac{1\text{ mol S}}{32.07\text{ g}}}$ mol S 1 mol S = 32.07 g
Solution:	$57.8\ \cancel{\text{g}}\text{ S} \times \frac{1\text{ mol}}{32.07\ \cancel{\text{g}}}$ $= 1.80\text{ mol S}$
Check:	Since the given amount is much less than 1 mol S, the number makes sense.

Practice—Calculate the Mass of Carbon 2.21×10^{-3} moles of Pencil Lead.

Given: **Find:**	2.21×10^{-3} moles mass of Carbon
Solution Map: **Relationships:**	mol C $\xrightarrow{\frac{12.01\text{ g}}{1\text{ mol}}}$ g C 1 mol C = 12.01 g
Solution:	$2.21 \times 10^{-3}\ \cancel{\text{mol C}} \times \frac{12.01\text{ g}}{1\ \cancel{\text{mol}}}$ $= 0.0265\text{ g C}$
Check:	Since the given amount is much less than 1 mol C, the number makes sense.

Mass and Atoms

Example 6.3—How Many Aluminum Atoms Are in a Can Weighing 16.2 g?

Given: **Find:**	16.2 g Al atoms Al
Solution Map:	g Al → mol Al → atoms Al $\frac{1\text{ mol}}{26.98\text{ g}}$ $\frac{6.022\times10^{23}\text{ atoms}}{1\text{ mol}}$
Relationships:	1 mol Al = 26.98 g, 1 mol = 6.022 x 10^{23}
Solution:	$16.2\ \cancel{\text{g Al}}\times\frac{1\ \cancel{\text{mol}}\text{ Al}}{26.98\ \cancel{\text{g Al}}}\times\frac{6.022\times10^{23}\text{ atoms}}{1\ \cancel{\text{mol}}}$ $=3.62\times10^{23}$ atoms Al
Check:	Since the given amount is much less than 1 mol Cu, the number makes sense.

Practice—What is the mass of 2.94 × 10^{22} atoms of Cu?

Given: **Find:**	2.94 × 10^{22} atoms Cu Mass of Cu
Solution Map:	atoms Cu → mol Cu → g Cu $\frac{1\text{ mol}}{6.022\times10^{23}\text{ atoms}}$ $\frac{63.55\text{ g}}{1\text{ mol}}$
Relationships:	1 mol Cu = 63.55 g, 1 mol = 6.022 x 10^{23}
Solution:	$2.94\times10^{22}\ \cancel{\text{atoms}}\text{ Cu}\times\frac{1\ \cancel{\text{mol}}}{6.022\times10^{23}\ \cancel{\text{atoms}}}\times\frac{63.55\text{ g Cu}}{1\ \cancel{\text{mol Cu}}}$ $=3.10$ g Cu
Check:	Since the given amount is much less than 1 mol Cu, the number makes sense.

Molar Mass of Compounds

Molar Mass of Compounds

- The relative weights of molecules can be calculated from atomic weights.

  Formula mass of 1 molecule of H_2O

  = 2(1.01 amu H) + 16.00 amu O = 18.02 amu.
- Since 1 mole of H_2O contains 2 moles of H and 1 mole of O.

  Molar mass of 1 mole H_2O

  = 2(1.01 g H) + 16.00 g O = 18.02 g.

Example 6.4—Calculate the Mass of 1.75 Mol of H_2O.

Given: **Find:**	1.75 mol H_2O g H_2O
Solution Map:	mol H_2O → g H_2O $\frac{18.02\text{ g}}{1\text{ mol }H_2O}$ H = 2× 1.01 amu O = 1× 16.00 amu H_2O = 18.02 amu
Relationships:	1 mol H_2O = 18.02 g
Solution:	$1.75\ \cancel{\text{mol}}\ H_2O\times\frac{18.02\text{ g}}{1\ \cancel{\text{mol}}}$ $=31.535\text{ g}=31.5\text{ g }H_2O$
Check:	Since the given amount is more than 1 mol, the mass being > 18 g makes sense.

Practice—How Many Moles Are in 50.0 g of PbO_2? (Pb = 207.2 amu, O = 16.00 amu)

Given: **Find:**	50.0 g mol PbO_2 moles PbO_2
Solution Map:	g PbO_2 → mol PbO_2 $\frac{1\text{ mol }PbO_2}{239.2\text{ g}}$ Pb = 1× 209.2 amu O = 2× 16.00 amu PbO_2 = 239.2 amu
Relationships:	1 mol PbO_2 = 239.2 g
Solution:	$50.0\ \cancel{\text{g}}\ PbO_2\times\frac{1\text{ mol}}{239.2\ \cancel{\text{g}}}$ $=0.20903\text{ mol}=0.209\text{ mol }PbO_2$
Check:	Since the given amount is less than 239.2 g, the moles being < 1 makes sense.

Practice—How Many Formula Units Are in 50.0 g of PbO_2? (PbO_2 = 239.2 amu)

Given: **Find:**	50.0 g PbO_2 formula units PbO_2
Solution Map:	g PbO_2 → mol PbO_2 → units PbO_2 $\frac{1\text{ mol}}{239.2\text{ g}}$ $\frac{6.022\times10^{23}\text{ molecules}}{1\text{ mol}}$
Relationships:	1 mol PbO_2 = 239.2 g,1 mol = 6.022 x 10^{23}
Solution:	$50.0\ \cancel{\text{g}\ PbO_2}\times\frac{1\ \cancel{\text{mol}}\ PbO_2}{239.2\ \cancel{\text{g}\ PbO_2}}\times\frac{6.022\times10^{23}\text{ units}}{1\ \cancel{\text{mol}}}$ $=1.26\times10^{23}$ units PbO_2
Check:	Since the given amount is much less than 1 mol PbO_2, the number makes sense.

Example 6.5—What Is the Mass of 4.78 x 10^{24} NO_2 Molecules?

Given: **Find:**	4.78 x 10^{24} NO_2 molecules g NO_2
Solution Map:	molecules → mol NO_2 → g NO_2 $\frac{1\text{ mol }NO_2}{6.022\times10^{23}\text{ molec}}$ $\frac{46.01\text{ g}}{1\text{ mol}}$ N = 1× 14.01 amu O = 2× 16.00 amu NO_2 = 46.01 amu
Relationships:	1 mol NO_2 = 46.01 g, 1 mol = 6.022 x 10^{23}
Solution:	$4.78\times10^{24}\ \cancel{\text{molec}}\ NO_2\times\frac{1\ \cancel{\text{mol}}}{6.022\times10^{23}\ \cancel{\text{molec}}}\times\frac{46.01\text{ g}}{1\ \cancel{\text{mol}}\ NO_2}$ $=365\text{ g }NO_2$
Check:	Since the given amount is more than Avogadro's number, the mass > 46 g makes sense.

Chemical Formulas as Conversion Factors

- 1 spider ≡ 8 legs.
- 1 chair ≡ 4 legs.
- 1 H_2O molecule ≡ 2 H atoms ≡ 1 O atom.

Counting Parts

- If we know how many parts are in the whole unit, by counting the number of whole units, we can effectively count the parts.
- For example, when all the desks in the room have 4 legs, if there are 30 desks in the room, there will be 120 legs (4 x 30).
- Since every H_2O molecule has 2 H atoms, in 100 H_2O molecules, there are 200 H atoms.
- In 1 mole of H_2O molecules, there are 2 moles of H atoms.

Mole Relationships in Chemical Formulas

- Since we count atoms and molecules in mole units, we can find the number of moles of a constituent element if we know the number of moles of the compound.

Moles of compound	Moles of constituents
1 mol NaCl	1 mol Na, 1 mol Cl
1 mol H_2O	2 mol H, 1 mol O
1 mol $CaCO_3$	1 mol Ca, 1 mol C, 3 mol O
1 mol $C_6H_{12}O_6$	6 mol C, 12 mol H, 6 mol O

Example 6.6—Calculate the Moles of Oxygen in 1.7 Moles of $CaCO_3$.

Given: **Find:**	1.7 mol $CaCO_3$ mol O
Solution Map:	mol $CaCO_3$ → mol O $\frac{3\text{ mol O}}{1\text{ mol }CaCO_3}$
Relationships:	1 mol $CaCO_3$ = 3 mol O
Solution:	$1.7\ \cancel{\text{mol}\ CaCO_3}\times\frac{3\text{ mol O}}{1\ \cancel{\text{mol}\ CaCO_3}}$ $=5.1\text{ mol O}$
Check:	Since there are multiple moles of O in every mole of $CaCO_3$, the number makes sense.

Example 6.7—Find the Mass of Carbon in 55.4 g $C_{10}H_{14}O$.

Given: **Find:**	55.4 g $C_{10}H_{14}O$ g C
Solution Map:	g $C_{10}H_{14}O$ → mol $C_{10}H_{14}O$ → mol C → g C $\frac{1\text{ mol}}{150.2\text{ g}}$ $\frac{10\text{ mol C}}{1\text{ mol }C_{10}H_{14}O}$ $\frac{12.01\text{ g}}{1\text{ mol}}$ C = 10× 12.01 amu H = 14× 1.01 amu O = 1× 16.00 amu $C_{10}H_{14}O$ = 150.2 amu
Relationships:	1 mol $C_{10}H_{14}O$ = 150.2 g, 1 mol C = 12.01 g, 10 mol C : 1 mol $C_{10}H_{14}O$
Solution:	$55.4\ \cancel{\text{g}}\ C_{10}H_{14}O\times\frac{1\ \cancel{\text{mol}}\ C_{10}H_{14}O}{150.2\ \cancel{\text{g}}}\times\frac{10\ \cancel{\text{mol}}\text{ C}}{1\ \cancel{\text{mol}}\ C_{10}H_{14}O}\times\frac{12.01\text{ g C}}{1\ \cancel{\text{mol}}\text{ C}}=44.3\text{ g C}$
Check:	Since the amount of C is less than the amount of $C_{10}H_{14}O$, the answer makes sense.

Practice—Find the Mass of Sodium in 6.2 g of NaCl, Continued

Given: **Find:**	6.2 g NaCl g Na
Solution Map:	g NaCl → mol NaCl → mol Na → g Na $\frac{1\text{ mol}}{58.44\text{ g}}$ $\frac{1\text{ mol Na}}{1\text{ mol NaCl}}$ $\frac{22.99\text{ g}}{1\text{ mol}}$ Na = 1× 22.99 amu Cl = 1× 35.45 amu NaCl = 58.44 amu
Relationships:	1 mol NaCl = 58.44 g, 1 mol Na = 22.99 g, 1 mol Na : 1 mol NaCl
Solution:	$6.2\ \cancel{\text{g}}\text{ NaCl}\times\frac{1\ \cancel{\text{mol NaCl}}}{58.44\ \cancel{\text{g}}}\times\frac{1\ \cancel{\text{mol Na}}}{1\ \cancel{\text{mol NaCl}}}\times\frac{22.99\text{ g Na}}{1\ \cancel{\text{mol Na}}}=2.4\text{ g Na}$
Check:	Since the amount of Na is less than the amount of NaCl, the answer makes sense.

Percent Composition

Percent Composition

- Percentage of each element in a compound.
  - ✓ By mass.
- Can be determined from:
  - ✓ The formula of the compound.
  - ✓ The experimental mass analysis of the compound.
- The percentages may not always total to 100% due to rounding.

$$\text{Percentage}=\frac{\text{mass of element }X\text{ in }1\text{ mol}}{\text{mass of }1\text{ mol of the compound}}\times100\%$$

$$\text{Percentage}=\frac{\text{part}}{\text{whole}}\times100\%$$

Example 6.9—Find the Mass Percent of Cl in $C_2Cl_4F_2$.

Given:	$C_2Cl_4F_2$
Find:	% Cl by mass
Solution Map:	$\text{Mass \% Cl} = \frac{4\times \text{molar mass Cl}}{\text{molar mass } C_2Cl_4F_2}\times 100\%$
Relationships:	$\text{Mass \% element } X = \frac{\text{mass element } X \text{ in 1 mol}}{\text{mass 1 mol of compound}}\times 100\%$
Solution:	$4\times\text{molar mass Cl} = 4(35.45\text{ g/mol}) = 141.8\text{ g/mol}$ $\text{molar mass } C_2Cl_4F_2 = 2(12.01) + 4(35.45) + 2(19.00) = 203.8\text{ g/mol}$ $\text{Mass \% Cl} = \frac{141.8\cancel{\text{ g/mol}}}{203.8\cancel{\text{ g/mol}}}\times 100\% = 69.58\%$
Check:	Since the percentage is less than 100 and Cl is much heavier than the other atoms, the number makes sense.

Mass Percent as a Conversion Factor

- The mass percent tells you the mass of a constituent element in 100 g of the compound.
  - ✓The fact that NaCl is 39% Na by mass means that 100 g of NaCl contains 39 g Na.
- This can be used as a conversion factor.
  - ✓100 g NaCl ≡ 39 g Na

$$\text{g NaCl}\times\frac{39\text{ g Na}}{100\text{ g NaCl}} = \text{g Na} \qquad \text{g Na}\times\frac{100\text{ g NaCl}}{39\text{ g Na}} = \text{g NaCl}$$

Empirical Formula

Empirical Formulas

- The simplest, whole-number ratio of atoms in a molecule is called the **empirical formula**.
  - ✓Can be determined from percent composition or combining masses.
- The molecular formula is a multiple of the empirical formula.

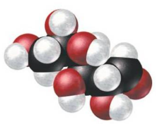
$$\%\text{ A} \xrightarrow{100\text{g}} \text{mass A (g)} \xrightarrow{MM_A} \text{moles A}$$
$$\%\text{ B} \xrightarrow{100\text{g}} \text{mass B (g)} \xrightarrow{MM_B} \text{moles B}$$
$$\rightarrow \frac{\text{moles A}}{\text{moles B}}$$

Empirical Formulas, Continued

Hydrogen Peroxide
Molecular formula = H_2O_2
Empirical formula = HO

Benzene
Molecular formula = C_6H_6
Empirical formula = CH

Glucose
Molecular formula = $C_6H_{12}O_6$
Empirical formula = CH_2O



Practice—Determine the Empirical Formula of Benzopyrene, $C_{20}H_{12}$, Continued

- Find the greatest common factor (GCF) of the subscripts.
  - 20 factors = (10 x 2), (5 x 4)
  - 12 factors = (6 x 2), (4 x 3)
  - GCF = 4
- Divide each subscript by the GCF to get the empirical formula.
  - $C_{20}H_{12} = (C_5H_3)_4$
  - Empirical formula = C_5H_3

Finding an Empirical Formula From Percent Composition

1. Convert the percentages to grams.
   a. Skip if already grams.
2. Convert grams to moles.
   a. Use molar mass of each element.
3. Write a pseudoformula using moles as subscripts.
4. Divide all by smallest number of moles.
5. Multiply all mole ratios by number to make all whole numbers, if necessary.
   a. If ratio 0.5, multiply all by 2; if ratio 0.33 or 0.67, multiply all by 3, etc.
   b. Skip if already whole numbers after Step 4.

Example 6.11—Finding an Empirical Formula from Experimental Data

Example:

- A laboratory analysis of aspirin determined the following mass percent composition. Find the empirical formula.
  - C = 60.00%
  - H = 4.48%
  - O = 35.53%

Example:
Find the empirical formula of aspirin with the given mass percent composition.

- Write down the given quantity and its units.
  - Given: C = 60.00%
  - H = 4.48%
  - O = 35.53%

Therefore, in 100 g of aspirin there are 60.00 g C, 4.48 g H, and 35.53 g O.

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 60.00 g C, 4.48 g H, 35.53 g O

- Write down the quantity to find and/or its units.
  - Find: empirical formula, $C_xH_yO_z$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 60.00 g C, 4.48 g H, 35.53 g O
Find: empirical formula, $C_xH_yO_z$

- Collect needed conversion factors:
  - 1 mole C = 12.01 g C
  - 1 mole H = 1.01 g H
  - 1 mole O = 16.00 g O

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 60.00 g C, 4.48 g H, 35.53 g O
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g; 1 mol H = 1.01 g; 1 mol O = 16.00 g

- Write a solution map:

g C → mol C
g H → mol H
g O → mol O
→ pseudo-formula $\xrightarrow{\text{mole ratio}}$ $\xrightarrow{\text{whole number ratio}}$ empirical formula

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 60.00 g C, 4.48 g H, 35.53 g O
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g
Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓Calculate the moles of each element.

$$60.00\cancel{\text{ g C}}\times\frac{1\text{ mol C}}{12.01\cancel{\text{ g C}}} = 4.996\text{ mol C}$$
$$4.48\cancel{\text{ g H}}\times\frac{1\text{ mol H}}{1.01\cancel{\text{ g H}}} = 4.44\text{ mol H}$$
$$35.53\cancel{\text{ g O}}\times\frac{1\text{ mol O}}{16.00\cancel{\text{ g O}}} = 2.221\text{ mol O}$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: 4.996 mol C, 4.44 mol H, 2.221 mol O
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g
Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓Write a pseudoformula.

$$C_{4.996}H_{4.44}O_{2.221}$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: $C_{4.996}H_{4.44}O_{2.221}$
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g
Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓Find the mole ratio by dividing by the smallest number of moles.

$$C_{\frac{4.996}{2.221}}H_{\frac{4.44}{2.221}}O_{\frac{2.221}{2.221}}$$

$$C_{2.25}H_2O_1$$

Example:
Find the empirical formula of aspirin with the given mass percent composition.

Information:
Given: $C_{2.25}H_2O_1$
Find: empirical formula, $C_xH_yO_z$
Conversion Factors:
1 mol C = 12.01 g;
1 mol H = 1.01 g; 1 mol O = 16.00 g
Solution Map: g C,H,O → mol C,H,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓ Multiply subscripts by factor to give whole number.

$$\{C_{2.25}H_2O_1\} \text{ x } 4$$

$$C_9H_8O_4$$

Example 6.12—Finding an Empirical Formula from Experimental Data

Example:
- A 3.24-g sample of titanium reacts with oxygen to form 5.40 g of the metal oxide. What is the formula of the oxide?

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

- Write down the given quantity and its units.

Given: Ti = 3.24 g
compound = 5.40 g

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 3.24 g Ti, 5.40 g compound

- Write down the quantity to find and/or its units.

Find: empirical formula, Ti_xO_y

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 3.24 g Ti, 5.40 g compound
Find: empirical formula, Ti_xO_y

- Collect needed conversion factors:

1 mole Ti = 47.88 g Ti
1 mole O = 16.00 g O

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 3.24 g Ti, 5.40 g compound
Find: empirical formula, Ti_xO_y
Conversion Factors:
1 mol Ti = 47.88 g;1 mol O = 16.00 g

- Write a solution map:

g Ti → mol Ti
g O → mol O
→ pseudo-formula $\xrightarrow{\text{mole ratio}}$ $\xrightarrow{\text{whole number ratio}}$ empirical formula

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 3.24 g Ti, 5.40 g compound
Find: empirical formula, Ti_xO_y
Conversion Factors:
1 mol Ti= 47.88 g;1 mol O= 16.00 g
Solution Map: g Ti,O → mol Ti,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓ Calculate the mass of each element.

5.40 g compound − 3.24 g Ti = 2.6 g O

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 3.24 g Ti, 2.16 g O
Find: empirical formula, Ti_xO_y
Conversion Factors:
1 mol Ti= 47.88 g;1 mol O= 16.00 g
Solution Map: g Ti,O → mol Ti,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓ Calculate the moles of each element.

$$3.24\,\cancel{\text{g Ti}} \times \frac{1\,\text{mol Ti}}{47.88\,\cancel{\text{g Ti}}} = 0.0677\text{ mol Ti}$$

$$2.16\,\cancel{\text{g O}} \times \frac{1\,\text{mol O}}{16.00\,\cancel{\text{g O}}} = 0.135\text{ mol O}$$

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 0.0677 mol Ti, 0.135 mol O
Find: empirical formula, Ti_xO_y
Conversion Factors:
1 mol Ti= 47.88 g;1 mol O= 16.00 g
Solution Map: g Ti,O → mol Ti,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓ Write a pseudoformula.

$$Ti_{0.0677}O_{0.135}$$

Example:
Find the empirical formula of oxide of titanium with the given elemental analysis.

Information:
Given: 0.0677 mol Ti, 0.135 mol O
Find: empirical formula, Ti_xO_y
Conversion Factors:
1 mol Ti= 47.88 g;1 mol O= 16.00 g
Solution Map: g Ti,O → mol Ti,O → mol ratio → empirical formula

- Apply the solution map:
  - ✓ Find the mole ratio by dividing by the smallest number of moles.

$$Ti_{\frac{0.0677}{0.0677}}O_{\frac{0.135}{0.0677}}$$

$$Ti_1O_2$$

Practice—Determine the Empirical Formula of Stannous Fluoride, which Contains 75.7% Sn (118.70) and the Rest Fluorine (19.00).

Practice—Determine the Empirical Formula of Stannous Fluoride, which Contains 75.7% Sn (118.70) and the Rest Fluorine (19.00), Continued.

Given: 75.7% Sn, (100 – 75.3) = 24.3% F ∴
in 100 g stannous fluoride there are 75.7 g Sn and 24.3 g F.
Find: Sn_xF_y
Conversion Factors: 1 mol Sn = 118.70 g; 1 mol F = 19.00 g
Solution Map:

g Sn → mol Sn
g F → mol F
→ pseudo-formula $\xrightarrow{\text{mole ratio}}$ $\xrightarrow{\text{whole number ratio}}$ empirical formula

Practice—Determine the Empirical Formula of Stannous Fluoride, which Contains 75.7% Sn (118.70) and the Rest Fluorine (19.00), Continued.

Apply solution map:

$$75.7\,\cancel{\text{g Sn}} \times \frac{1\,\text{mol Sn}}{118.70\,\cancel{\text{g}}} = 0.638\text{ mol Sn}$$

$$24.3\,\cancel{\text{g F}} \times \frac{1\,\text{mol F}}{19.00\,\cancel{\text{g}}} = 1.28\text{ mol F}$$

$$Sn_{0.638}F_{1.28}$$

$$Sn_{\frac{0.638}{0.638}}F_{\frac{1.28}{0.638}} = Sn_1F_2$$

$$SnF_2$$

Practice—Determine the Empirical Formula of Hematite, which Contains 72.4% Fe (55.85) and the Rest Oxygen (16.00).

Practice—Determine the Empirical Formula of Hematite, which Contains 72.4% Fe (55.85) and the Rest Oxygen (16.00), Continued.

Given: 72.4% Fe, (100 – 72.4) = 27.6% O ∴
in 100 g hematite there are 72.4 g Fe and 27.6 g O.
Find: Fe_xO_y
Conversion Factors: 1 mol Fe = 55.85 g; 1 mol O = 16.00 g
Solution Map:

g Fe → mol Fe
g O → mol O
→ pseudo-formula $\xrightarrow{\text{mole ratio}}$ $\xrightarrow{\text{whole number ratio}}$ empirical formula

Practice—Determine the Empirical Formula of Hematite, which Contains 72.4% Fe (55.85) and the Rest Oxygen (16.00), Continued.

Apply solution map:

$$72.4\ \cancel{g\ Fe} \times \frac{1\ mol\ Fe}{55.85\ \cancel{g}} = 1.30\ mol\ Fe$$

$$26.7\ \cancel{g\ O} \times \frac{1\ mol\ O}{16.00\ \cancel{g}} = 1.73\ mol\ O$$

$$Fe_{1.30}O_{1.73}$$

$$Fe_{\frac{1.30}{1.30}}O_{\frac{1.73}{1.30}} = Fe_1O_{1.33}$$

$$\left(Fe_1O_{1.33}\right) \times 3 = Fe_3O_4$$

Molecular Formulas From Empirical Formulas

All These Molecules Have the Same Empirical Formula. How Are the Molecules Different?

Name	Molecular Formula	Empirical Formula	
Glyceraldehyde	$C_3H_6O_3$	CH_2O	
Erythrose	$C_4H_8O_4$	CH_2O	
Arabinose	$C_5H_{10}O_5$	CH_2O	
Glucose	$C_6H_{12}O_6$	CH_2O	

All These Molecules Have the Same Empirical Formula. How Are the Molecules Different?, Continued

Name	Molecular Formula	Empirical Formula	Molar Mass, g
Glyceraldehyde	$C_3H_6O_3$	CH_2O	90
Erythrose	$C_4H_8O_4$	CH_2O	120
Arabinose	$C_5H_{10}O_5$	CH_2O	150
Glucose	$C_6H_{12}O_6$	CH_2O	180

Molecular Formulas

- The molecular formula is a multiple of the empirical formula.
- To determine the molecular formula, you need to know the empirical formula and the molar mass of the compound.

$$\frac{\text{Molar mass}_{\text{real formula}}}{\text{Molar mass}_{\text{empirical formula}}} = \text{Factor used to multiply subscripts}$$

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g/mol and an Empirical Formula of C_5H_8.

1. Determine the empirical formula.
   - ✓ May need to calculate it as previous.

   C_5H_8
2. Determine the molar mass of the empirical formula.

   5 C = 60.05 g/mol, 8 H = 8.064 g/mol

   C_5H_8 = 68.11 g/mol

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g/mol and an Empirical Formula of C_5H_8, Continued.

3. Divide the given molar mass of the compound by the molar mass of the empirical formula.
   - ✓ Round to the nearest whole number.

$$\frac{204\ \cancel{g/mol}}{68.11\ \cancel{g/mol}} = 3$$

Example—Determine the Molecular Formula of Cadinene if it has a Molar Mass of 204 g/mol and an Empirical Formula of C_5H_8, Continued.

4. Multiply the empirical formula by the factor above to give the molecular formula.

$(C_5H_8)_3 = C_{15}H_{24}$

Practice—Benzopyrene has a Molar Mass of 252 g and an Empirical Formula of C_5H_3. What is its Molecular Formula? (C = 12.01, H=1.01), Continued

C_5 = 5 × (12.01 g/mol) = 60.05 g/mol

$\underline{H_3 = 3 \times (1.01\ g/mol) = 3.03\ g/mol}$

C_5H_3 = 63.08 g/mol

$$n = \frac{252\ \cancel{g/mol}}{63.08\ \cancel{g/mol}} = 4$$

Molecular formula = $(C_5H_3)_4 = C_{20}H_{12}$

Practice—Determine the Molecular Formula of Nicotine, which has a Molar Mass of 162 g/mol and is 74.0% C, 8.7% H, and the Rest N, Continued

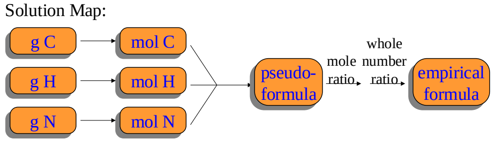
Given: 74.0% C, 8.7% H, {100% – (74.0% + 8.7%)} = 17.3% N ∴ in 100 g nicotine there are 74.0 g C, 8.7 g H, and 17.3 g N.

Find: $C_xH_yN_z$

Conversion Factors:

1 mol C = 12.01 g; 1 mol H = 1.01 g; 1 mol N = 14.01 g

Solution Map:



Practice—Determine the Molecular Formula of Nicotine, which has a Molar Mass of 162 g/mol and is 74.0% C, 8.7% H, and the Rest N, Continued.

Apply solution map:

$$74.0\ \cancel{g}\ C \times \frac{1\ mol\ C}{12.01\ \cancel{g}} = 6.16\ mol\ C$$

$$8.7\ \cancel{g}\ H \times \frac{1\ mol\ H}{1.01\ \cancel{g}} = 8.6\ mol\ H$$

$$17.3\ \cancel{g}\ N \times \frac{1\ mol\ N}{14.01\ \cancel{g}} = 1.23\ mol\ N$$

$$C_{6.16}H_{8.6}N_{1.23}$$

$$C_{\frac{6.16}{1.23}}H_{\frac{8.6}{1.23}}N_{\frac{1.23}{1.23}} = C_5H_7N$$

C_5 = 5(12.01 g/mol) = 60.05 g/mol

N_1 = 1(14.01 g/mol) = 14.01 g/mol

$\underline{H_7 = 7(1.01\ g/mol) = 7.07\ g/mol}$

C_5H_7N = 81.13 g/mol

$$\frac{162\ \cancel{g/mol}}{81.13\ \cancel{g/mol}} = 2$$

$(C_5H_7N)_2 = C_{10}H_{14}N_2$