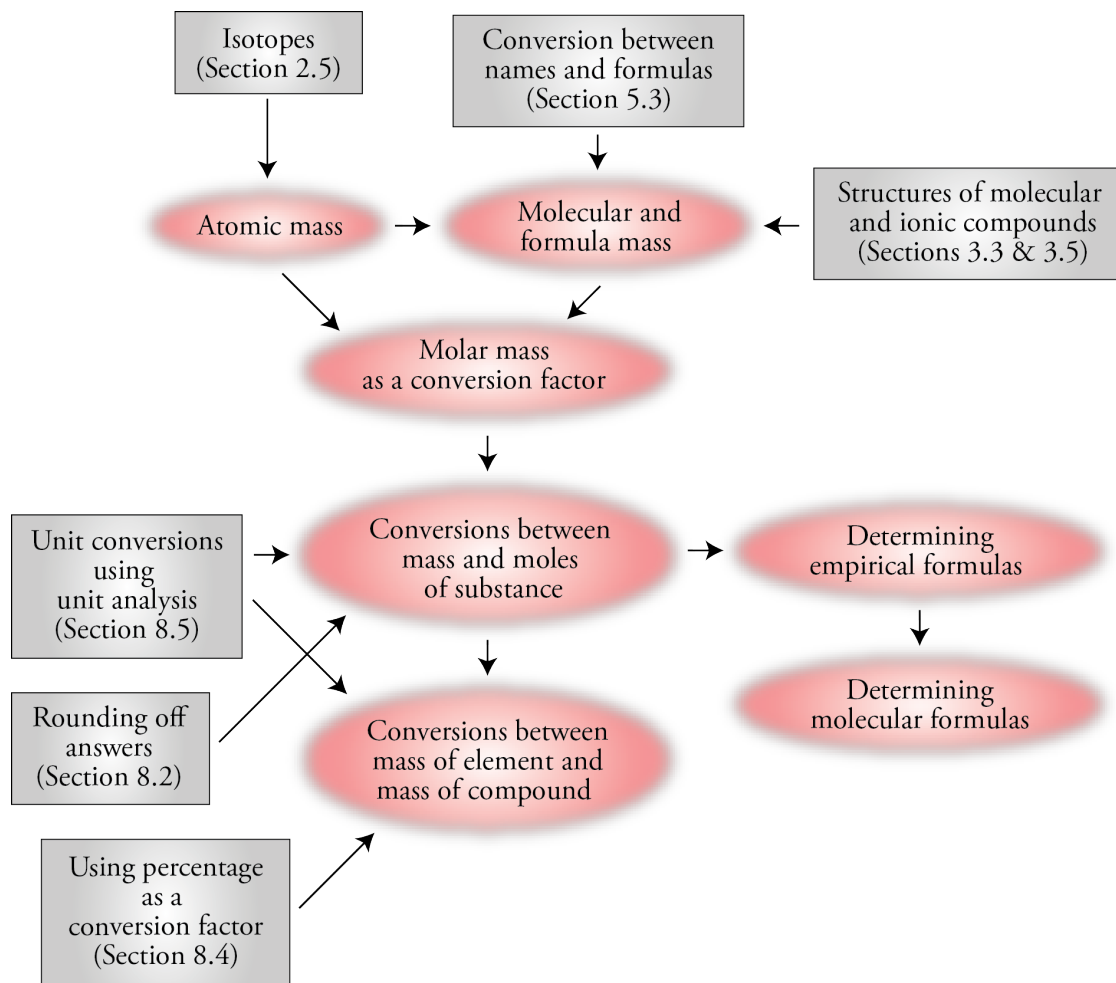


Chapter 9

Chemical Calculations and Chemical Formulas

An Introduction to Chemistry
by Mark Bishop

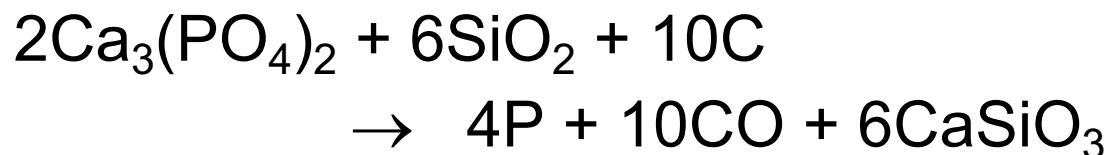
Chapter Map



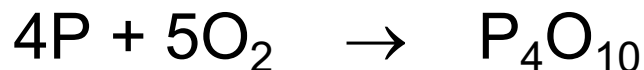
Making Phosphoric Acid

- Furnace Process for making H_3PO_4 to be used to make fertilizers, detergents, and pharmaceuticals.

- React phosphate rock with sand and coke at 2000 °C.



- React phosphorus with oxygen to get tetraphosphorus decoxide.



- React tetraphosphorus decoxide with water to make phosphoric acid.



Sample Calculations (1)

- What is the maximum mass of P_4O_{10} that can be formed from 1.09×10^4 kg P?
- Beginning of unit analysis setup.

$$? \text{ kg } P_4O_{10} = 1.09 \times 10^4 \text{ kg } P \left(\frac{\quad}{1 \text{ kg}} \right)$$

- The formula for P_4O_{10} provides us with a conversion factor that converts from units of P to units of P_4O_{10} .

$$\frac{1 \text{ molecule } P_4O_{10}}{4 \text{ atoms } P}$$

Sample Calculations (2)

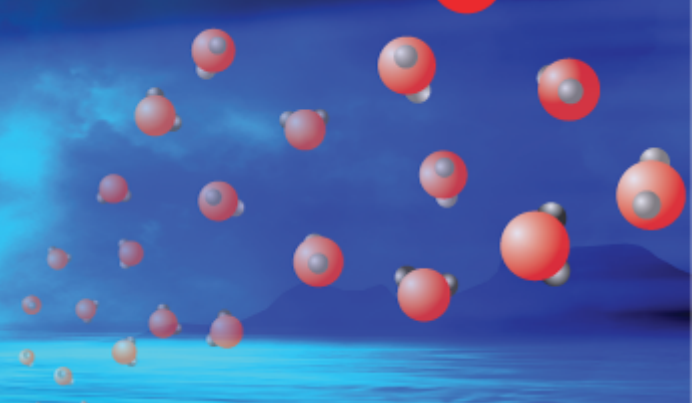
- What is the minimum mass of water that must be added to 2.50×10^4 kg P_4O_{10} to form phosphoric acid in the following reaction?



- The coefficients in the balanced equation provide us with a conversion factor that converts from units of P_4O_{10} to units of H_2O .

$$\frac{6 \text{ molecules } H_2O}{1 \text{ molecule } P_4O_{10}}$$

Goal: To develop conversion factors that will convert between a measurable property (mass) and number of particles



$$? \text{ kg P}_4\text{O}_{10} = 1.09 \times 10^4 \cancel{\text{ kg P}} \left(\frac{\quad}{1 \cancel{\text{ kg}}} \right)$$

Measurable Property 1



Number of Particles 1



Number of Particles 2



Measurable Property 2

Mass 1



Number of Particles 1



Number of Particles 2



Mass 2

Counting by Weighing for Nails

- **Step 1:** Choose an easily measurable property.
 - Mass for nails
- **Step 2:** Choose a convenient unit for measurement.
 - Pounds for nails

Counting by Weighing for Nails (cont)

- **Step 3:** If the measurable property is mass, determine the mass of the individual objects being measured.
 - Weigh 100 nails: 82 are 3.80 g, 14 are 3.70 g, and 4 are 3.60 g
- **Step 4:** If the objects do not all have the same mass, determine the weighted average mass of the objects.

$$0.82(3.80 \text{ g}) + 0.14(3.70 \text{ g}) + 0.04(3.60 \text{ g}) = 3.78 \text{ g}$$

Counting by Weighing for Nails (cont)

- **Step 5:** Use the conversion factor from the weighted average to make conversions between mass and number of objects.

$$? \text{ nails} = 218 \cancel{\text{ lb}} \cancel{\text{ nails}} \left(\frac{453.6 \cancel{\text{ g}}}{1 \cancel{\text{ lb}}} \right) \left(\frac{1 \text{ nail}}{3.78 \cancel{\text{ g}} \text{ nails}} \right) = 2.62 \times 10^4 \text{ nails}$$

Counting by Weighing for Nails (cont)

- **Step 6:** Describe the number of objects in terms of a collective unit, such as a dozen, a gross, or a ream.

$$\frac{? \text{ g nails}}{1 \text{ gross nails}} = \left(\frac{3.78 \text{ g nails}}{1 \text{ ~~nail~~}} \right) \left(\frac{144 \text{ ~~nails~~}}{1 \text{ gross nails}} \right) = \frac{544 \text{ g nails}}{1 \text{ gross nails}}$$

$$? \text{ gross nails} = 218 \text{ ~~lb nails~~} \left(\frac{453.6 \text{ ~~g}~~}{1 \text{ ~~lb}~~}} \right) \left(\frac{1 \text{ gross nails}}{544 \text{ ~~g nails~~}} \right) = 182 \text{ gross nails}$$

Counting by Weighing for Carbon Atoms



- **Step 1:** Choose an easily measurable property.
 - Mass for carbon atoms
- **Step 2:** Choose a convenient unit for measurement.
 - Atomic mass units (u) for carbon atoms
 - Atomic mass unit (u) = 1/12 the mass of a carbon-12 atom (with 6 p, 6 n, and 6 e⁻)

Counting by Weighing for Carbon Atoms (cont.)

- **Step 3:** If the measurable property is mass, determine the mass of the individual objects being measured.
 - For carbon: 98.90% are 12 u and 1.10% are 13.003355 u.
- **Step 4:** If the objects do not all have the same mass, determine the weighted average mass of the objects.
$$0.9890(12 \text{ u}) + 0.0110(13.003355 \text{ u}) = 12.011 \text{ u}$$

Counting by Weighing for Carbon Atoms (cont.)

- For two reasons, we will skip step 5 where we would have used the weighted average mass, 12.011 u per atom, as a conversion factor.
 - The first reason is that we don't measure mass in unified mass units.
 - The second reason is that if we used 12.011 u per atom as a conversion factor, we would get the actual number of atoms, which for any sample of carbon would be a huge and inconvenient number.

Counting by Weighing for Carbon Atoms (cont.)

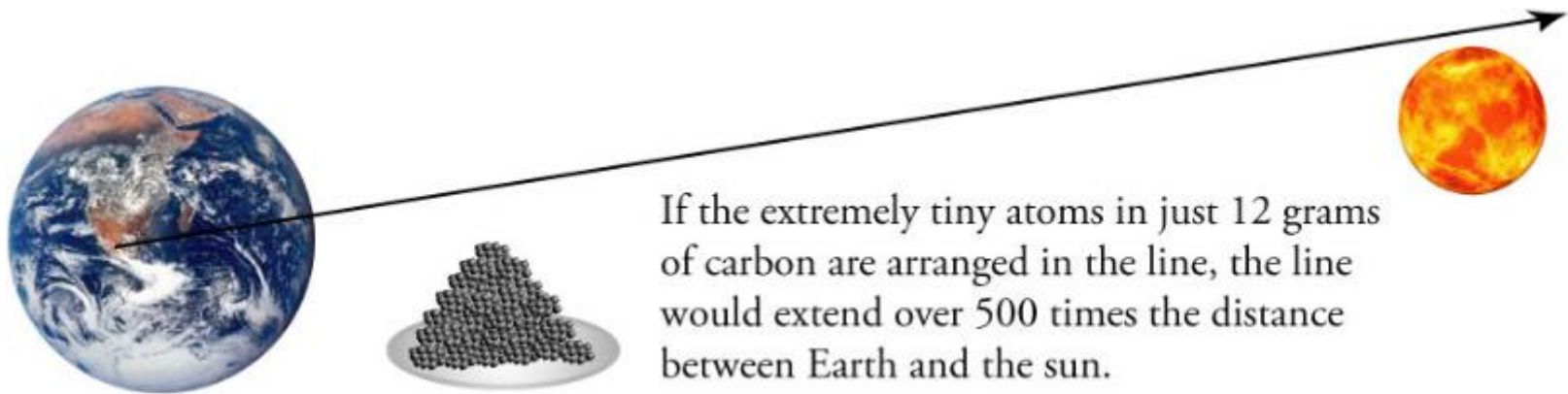
- We would rather have a conversion factor that has a more common mass unit, such as grams, and we would rather describe the number of atoms in terms of a collective unit, such as a dozen, a gross, or a ream.
- That collective unit is a mole.

Mole



- A ***mole*** (mol) is an amount of substance that contains the same number of particles as there are atoms in 12 g of carbon-12.
- To four significant figures, there are 6.022×10^{23} atoms in 12 g of carbon-12.
- Thus a mole of natural carbon is the amount of carbon that contains 6.022×10^{23} carbon atoms.
- The number 6.022×10^{23} is often called ***Avogadro's number***.

Avogadro's Number



If the extremely tiny atoms in just 12 grams of carbon are arranged in the line, the line would extend over 500 times the distance between Earth and the sun.

Molar Mass Development

From the definition of mole

$$\frac{12 \text{ g C-12}}{1 \text{ mol C-12}}$$

From relative atomic masses

$$\frac{12.011 \text{ g C}}{1 \text{ mol C}}$$

$$\frac{24.3050 \text{ g Mg}}{1 \text{ mol Mg}}$$

$$\frac{15.9994 \text{ g O}}{1 \text{ mol O}}$$

$$\frac{1.00794 \text{ g H}}{1 \text{ mol H}}$$

Molar Mass of Elements

- The atomic masses found on the periodic table can be used to get molar masses, which can be used to convert between grams and moles of any element.

$$\left(\frac{(\text{atomic mass}) \text{ g element}}{1 \text{ mol element}} \right)$$

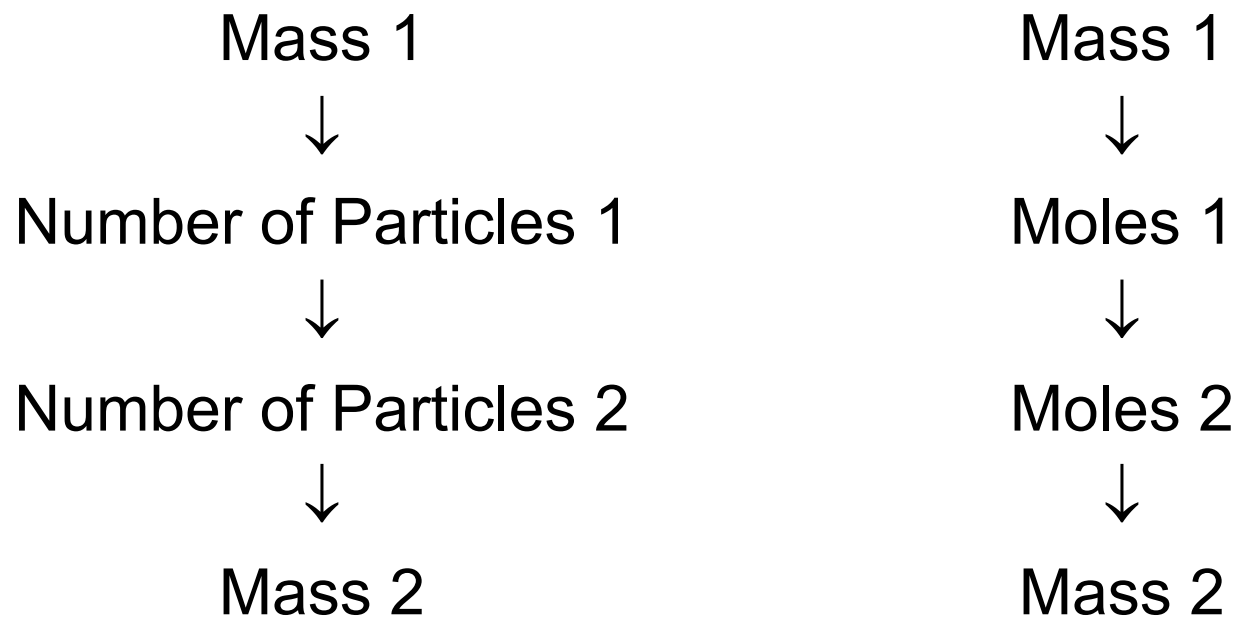
Example Calculations

- The masses of diamonds and other gemstones are measured in carats. There are exactly 5 carats per gram. How many moles of carbon atoms are in a 0.55 carat diamond? (Assume that the diamond is pure carbon.)

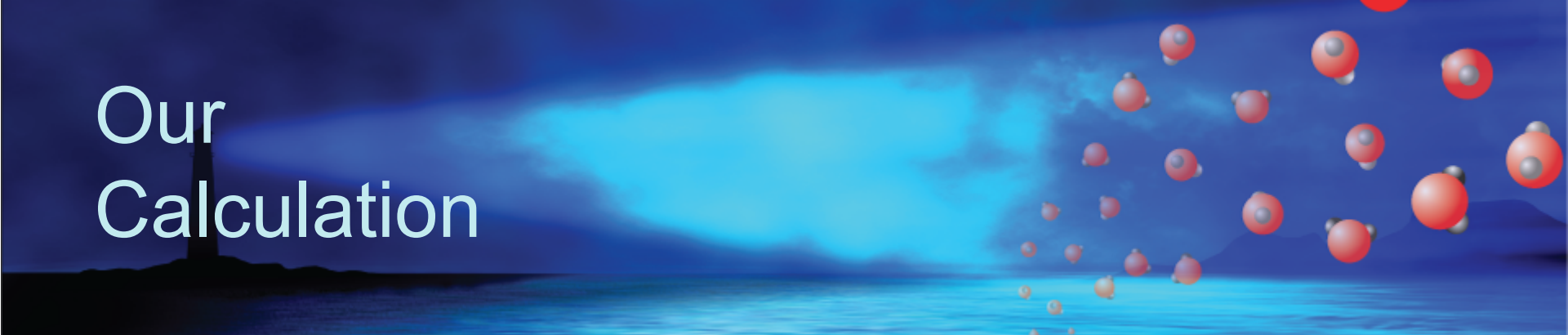
$$\begin{aligned} ? \text{ mol C} &= 0.55 \cancel{\text{carat C}} \left(\frac{1 \cancel{\text{g}}}{5 \cancel{\text{carat}}} \right) \left(\frac{1 \text{ mol C}}{12.011 \cancel{\text{g C}}} \right) \\ &= 9.2 \times 10^{-3} \text{ mol C} \left(\frac{6.022 \times 10^{23} \text{ C atoms}}{1 \text{ mol C}} \right) \\ &= 5.5 \times 10^{21} \text{ C atoms} \end{aligned}$$

Our Calculation

- What is the maximum mass of P_4O_{10} that can be formed from $1.09 \times 10^4 \text{ kg P}$?



Our Calculation



- What is the maximum mass of P_4O_{10} that can be formed from $1.09 \times 10^4 \text{ kg P}$?
- Here are the general steps for our calculation. We'll see how to do the first two steps in this lesson, and I'll tell you how to do the last step in another lesson.

Mass P \rightarrow moles P \rightarrow moles P_4O_{10} \rightarrow mass P_4O_{10}

Our Calculation – Step 1

- What is the maximum mass of P_4O_{10} that can be formed from 1.09×10^4 kg P?

Mass P \rightarrow moles P \rightarrow moles P_4O_{10} \rightarrow mass P_4O_{10}

- We can convert grams of P to moles of P using the molar mass of P, which comes from its atomic mass that is found on the periodic table.

$$\frac{30.9738 \text{ g P}}{1 \text{ mol P}} \quad \text{or} \quad \frac{1 \text{ mol P}}{30.9738 \text{ g P}}$$

Our Calculation – Step 1

- What is the maximum mass of P_4O_{10} that can be formed from 1.09×10^4 kg P?

Mass P \rightarrow moles P \rightarrow moles P_4O_{10} \rightarrow mass P_4O_{10}

- Before we can convert grams P to moles P, we need to convert kg to g.

Converts given mass
unit into grams.

$$? \text{ kg } P_4O_{10} = 1.09 \times 10^4 \text{ kg P} \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol P}}{30.9738 \text{ g P}} \right)$$

Converts grams of
element into moles.

Our Calculation

- The chemical formula provides a conversion factor for converting from moles of phosphorus atoms to moles of tetraphosphorus decoxide molecules in the second step of our calculation.

$$\text{If } \frac{1 \text{ molecule P}_4\text{O}_{10}}{4 \text{ atoms P}} \text{ then } \frac{1 \text{ mol P}_4\text{O}_{10}}{4 \text{ mol P}}$$

Our Calculation – Steps 1 and 2

- What is the maximum mass of P_4O_{10} that can be formed from 1.09×10^4 kg P?
- Here are the first two steps in our calculation.
- We'll see how to do the last step in another section.

Converts given mass
unit into grams.

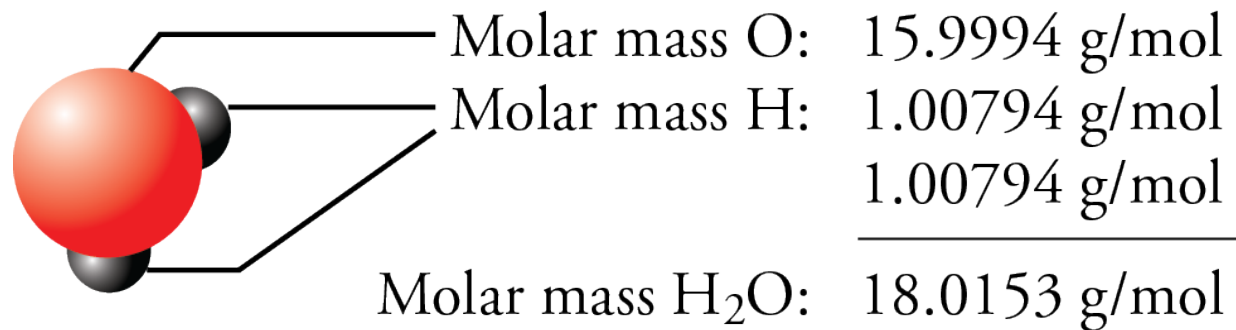
Converts moles of element
into moles of compound.

$$? \text{ kg } P_4O_{10} = 1.09 \times 10^4 \text{ kg } P \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol } P}{30.9738 \text{ g } P} \right) \left(\frac{1 \text{ mol } P_4O_{10}}{4 \text{ mol } P} \right)$$

Converts grams of
element into moles.

Molecular Mass

- Whole = sum of parts
- mass of a molecule = sum of the masses of the atoms in the molecule
- **molecular mass** = the sum of the atomic masses of the atoms in the molecule



Molar Mass For Molecular Compounds



- ***Molecular Mass*** = Sum of the atomic masses of atoms in one molecule

$$\left(\frac{(\text{molecular mass}) \text{ g molecular compound}}{1 \text{ mol molecular compound}} \right)$$

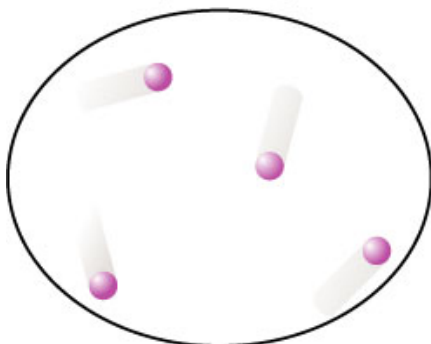
Formula Units



- A ***formula unit*** of a substance is the group represented by the substance's chemical formula, that is, a group containing the kinds and numbers of atoms or ions listed in the chemical formula.
- Formula unit is a general term that can be used in reference to elements, molecular compounds, or ionic compounds.

Formula Unit Examples

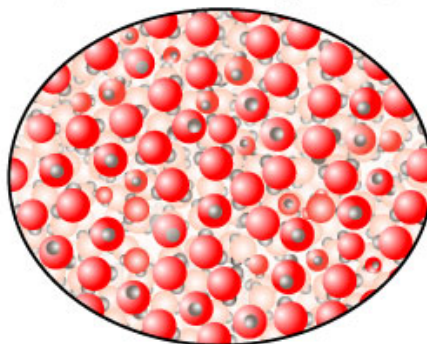
neon gas
(element)



A formula unit of neon contains one Ne atom.



liquid water
(molecular compound)

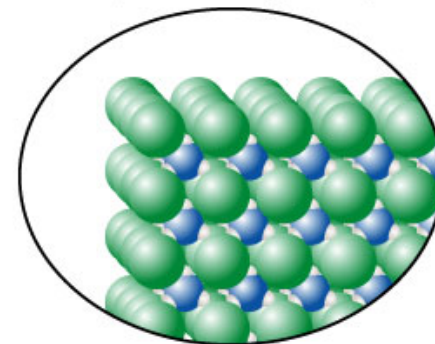


Liquid water is composed of discrete H₂O molecules.



A formula unit of water contains one oxygen atom and two hydrogen atoms.

ammonium chloride
(ionic compound)

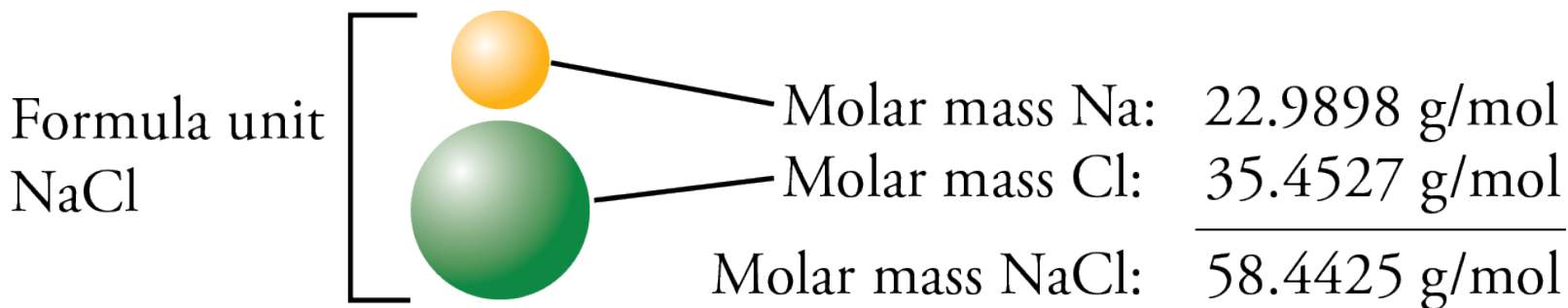


There are no separate ammonium chloride, NH₄Cl, molecules. Each ion is equally attracted to eight others. A formula unit of ammonium chloride contains one ammonium ion, NH₄⁺, and one chloride ion, Cl⁻, (or one nitrogen atom, four hydrogen atoms, and one chloride ion).



Formula Mass for Ionic Compounds

- Whole = sum of parts
- Mass of a formula unit = sum of the masses of the atoms in the formula unit
- **Formula mass** = the sum of the atomic masses of the atoms in the formula



Molar Mass For Ionic Compounds

- **Formula Mass** = Sum of the atomic masses of the atoms in a formula unit

$$\left(\frac{\text{(formula mass) g ionic compound}}{1 \text{ mol ionic compound}} \right)$$

Molar Mass Development

From the definition of an unified atomic mass unit, u $\frac{12 \text{ u C-12}}{1 \text{ atom C-12}}$

From the definition of mole $\frac{12 \text{ g C-12}}{1 \text{ mol C-12}}$

From relative atomic masses

$\frac{12.011 \text{ g C}}{1 \text{ mol C}}$	$\frac{24.3050 \text{ g Mg}}{1 \text{ mol Mg}}$	$\frac{15.9994 \text{ g O}}{1 \text{ mol O}}$	$\frac{1.00794 \text{ g H}}{1 \text{ mol H}}$
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From relative molecular masses $\frac{18.0153 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}}$

From relative formula masses $\frac{58.4425 \text{ g NaCl}}{1 \text{ mol NaCl}}$

General Conversions

Measurable property of substance 1



Moles of substance 1

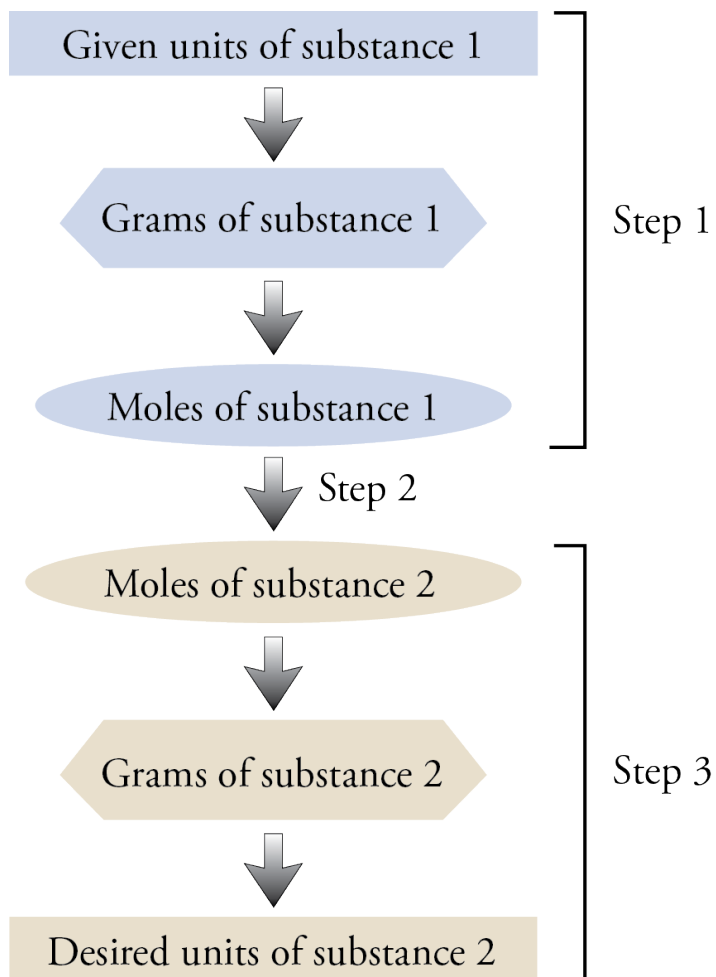


Moles of substance 2




Measurable property of substance 2

Units of One Substance to Units of Another



Study Sheets



- Write a description of the “tip-off” that helps you to recognize the type of problem the calculation represents.
- Write a description of the general procedure involved in the particular type of problem.
- Write an example of the type of calculation.

Sample Study Sheet: Converting Between Mass of Element and Mass of Compound Containing the Element



- **Tip-off:** When you analyze the type of unit you have and the type of unit you want, you recognize that you are converting between a unit associated with an element and a unit associated with a compound containing that element.

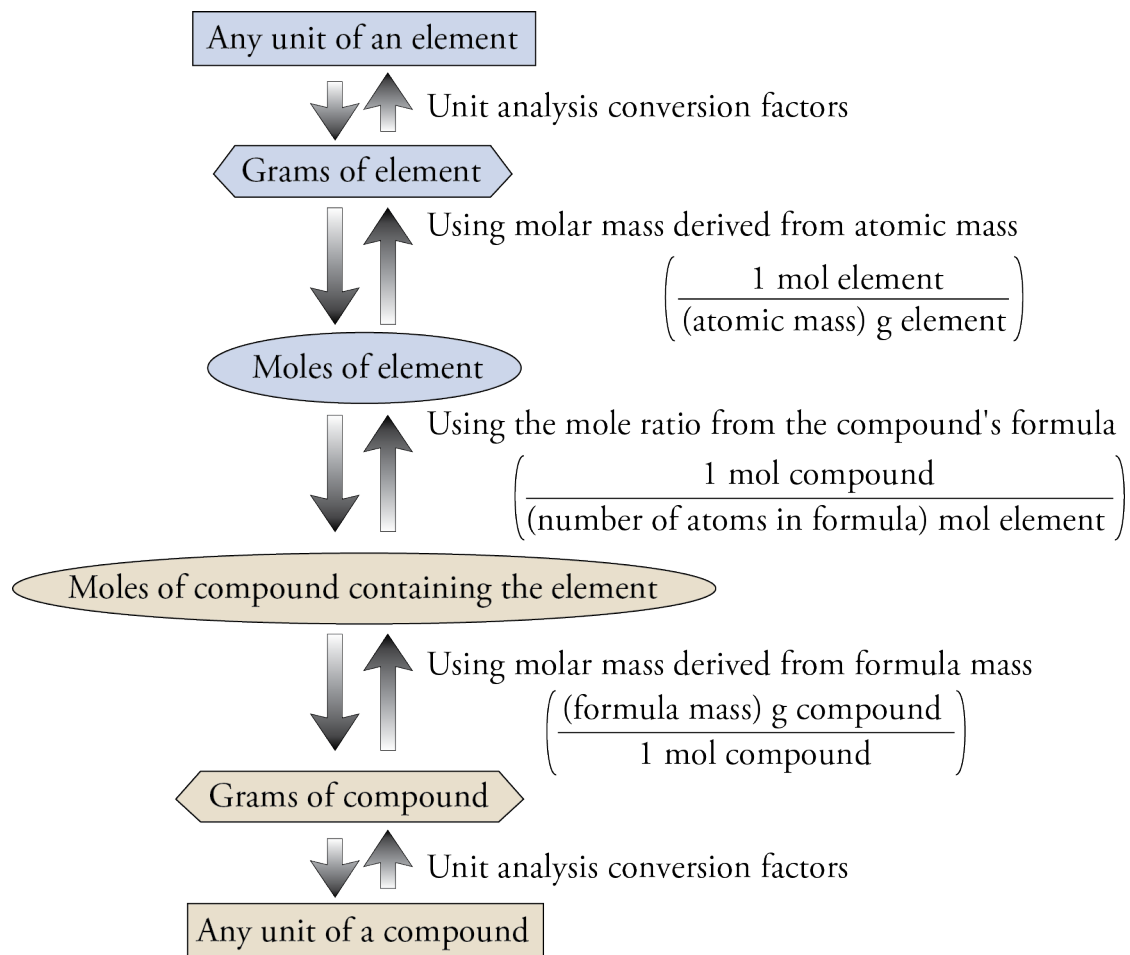
Sample Study Sheet (2)



- **General Steps**

- Convert the given unit to moles of the first substance.
- Convert moles of the first substance to moles of the second substance using the molar ratio derived from the formula for the compound.
- Convert moles of the second substance to the desired units of the second substance.

Units of Element to Units of Compound



Example Problem

Converts given mass
unit into grams.

Converts moles of element
into moles of compound.

Converts grams into
desired mass unit.

$$\begin{aligned}
 ? \text{ kg P}_4\text{O}_{10} &= 1.09 \times 10^4 \text{ kg P} \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol P}}{30.9738 \text{ g P}} \right) \left(\frac{1 \text{ mol P}_4\text{O}_{10}}{4 \text{ mol P}} \right) \left(\frac{283.889 \text{ g P}_4\text{O}_{10}}{1 \text{ mol P}_4\text{O}_{10}} \right) \left(\frac{1 \text{ kg}}{10^3 \text{ g}} \right) \\
 &= 2.50 \times 10^4 \text{ kg P}_4\text{O}_{10}
 \end{aligned}$$

Converts grams of element into moles.
Converts moles of compound into grams.

Empirical and Molecular Formulas



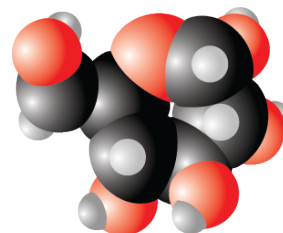
- When the subscripts in a chemical formula represent the simplest ratio of the kinds of atoms in the compound, the formula is called an ***empirical formula***.
 - Most ionic compounds are described with empirical formulas.
- A ***molecular formula*** describes the actual numbers of atoms of each element in a molecule.

Examples of Empirical and Molecular Formulas

- Hydrogen peroxide
 - Molecular formula – H_2O_2
 - Empirical formula – HO
- Glucose
 - Molecular formula – $\text{C}_6\text{H}_{12}\text{O}_6$
 - Empirical formula – CH_2O



hydrogen peroxide
molecular formula, H_2O_2 ,
empirical formula, HO



glucose
molecular formula, $\text{C}_6\text{H}_{12}\text{O}_6$,
empirical formula, CH_2O

Calculating Empirical Formulas



Step 1: If you are not given mass in grams for each element, convert the data you are given to grams of each element.

- This may involve simple unit conversions. For example, you may be given pounds or milligrams, which you convert to grams using unit analysis.
- Sometimes you are given the percentage of each element in the compound. Assume that you have 100 g of compound, and change the numbers for the percentages to grams.

Calculating Empirical Formulas

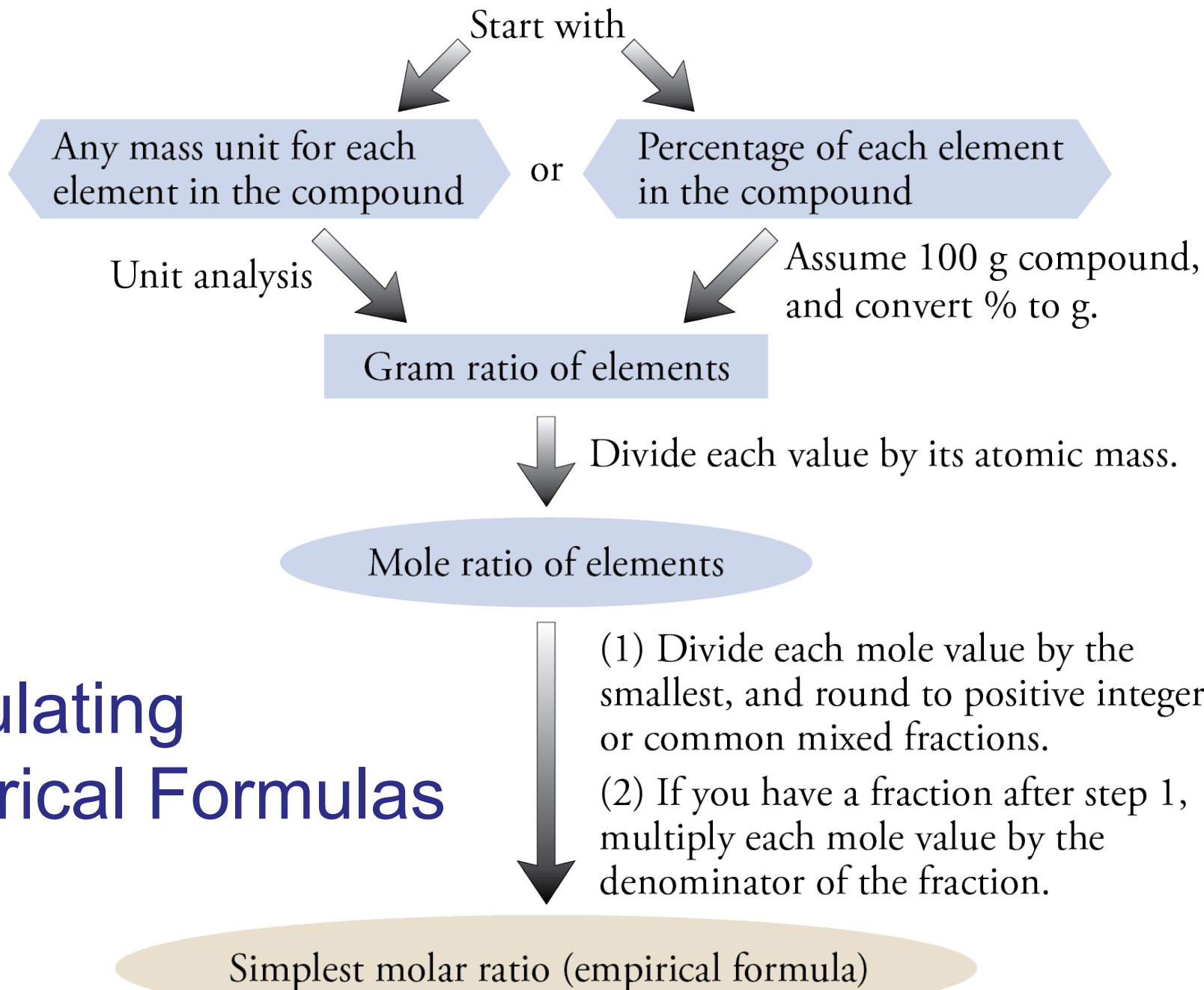


Step 2: Convert grams of each element to moles by dividing by the atomic mass of the element.

Step 3: Divide each mole value by the smallest and round your answers to whole numbers or common mixed fractions.

Step 4: If you have a fraction after the last step, multiply all the mole values by the denominator of the fraction.

Step 5: The resulting mole values correspond to the subscripts in the empirical formula.



Calculating Empirical Formulas

Example Empirical Formula Calculation

- An ionic compound used in the brewing industry to clean casks and vats and in the wine industry to kill undesirable yeasts and bacteria is composed of 35.172% potassium, 28.846% sulfur, and 35.982% oxygen. What is the empirical formula for this compound?
- **Step 1:** Convert percentages to a gram ratio of the elements by assuming 100 g.
35.172 g K : 28.846 g S : 35.982 g O

Example Empirical Formula Calculation

- An ionic compound used in the brewing industry to clean casks and vats and in the wine industry to kill undesirable yeasts and bacteria is composed of 35.172% potassium, 28.846% sulfur, and 35.982% oxygen. What is the empirical formula for this compound?
- **Step 2:** Convert grams of each element to moles by dividing by the atomic mass of the element.

$$? \text{ mol K} = 35.172 \text{ g K} \left(\frac{1 \text{ mol K}}{39.0983 \text{ g K}} \right) = 0.89958 \text{ mol K}$$

$$? \text{ mol S} = 28.846 \text{ g S} \left(\frac{1 \text{ mol S}}{32.066 \text{ g S}} \right) = 0.89958 \text{ mol S}$$

$$? \text{ mol O} = 35.982 \text{ g O} \left(\frac{1 \text{ mol O}}{15.9994 \text{ g O}} \right) = 2.2490 \text{ mol O}$$

Example Empirical Formula Calculation

- An ionic compound used in the brewing industry to clean casks and vats and in the wine industry to kill undesirable yeasts and bacteria is composed of 35.172% potassium, 28.846% sulfur, and 35.982% oxygen. What is the empirical formula for this compound?
- **Step 3:** Divide each mole value by the smallest and round your answers to whole numbers or common mixed fractions.

$$? \text{ mol K} = 35.172 \text{ g K} \left(\frac{1 \text{ mol K}}{39.0983 \text{ g K}} \right) = 0.89958 \text{ mol K} \div 0.89958 = 1 \text{ mol K}$$

$$? \text{ mol S} = 28.846 \text{ g S} \left(\frac{1 \text{ mol S}}{32.066 \text{ g S}} \right) = 0.89958 \text{ mol S} \div 0.89958 = 1 \text{ mol S}$$

$$? \text{ mol O} = 35.982 \text{ g O} \left(\frac{1 \text{ mol O}}{15.9994 \text{ g O}} \right) = 2.2490 \text{ mol O} \div 0.89958 \approx 2\frac{1}{2} \text{ mol O}$$

Example Empirical Formula Calculation

- An ionic compound used in the brewing industry to clean casks and vats and in the wine industry to kill undesirable yeasts and bacteria is composed of 35.172% potassium, 28.846% sulfur, and 35.982% oxygen. What is the empirical formula for this compound?
- **Step 4:** If you have a fraction after the last step, multiply all the mole values by the denominator of the fraction.

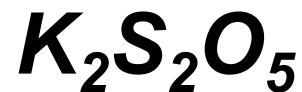
$$? \text{ mol K} = 35.172 \text{ g K} \left(\frac{1 \text{ mol K}}{39.0983 \text{ g K}} \right) = 0.89958 \text{ mol K} \div 0.89958 = 1 \text{ mol K} \times 2 \approx 2 \text{ mol K}$$

$$? \text{ mol S} = 28.846 \text{ g S} \left(\frac{1 \text{ mol S}}{32.066 \text{ g S}} \right) = 0.89958 \text{ mol S} \div 0.89958 = 1 \text{ mol S} \times 2 = 2 \text{ mole S}$$

$$? \text{ mol O} = 35.982 \text{ g O} \left(\frac{1 \text{ mol O}}{15.9994 \text{ g O}} \right) = 2.2490 \text{ mol O} \div 0.89958 \approx 2\frac{1}{2} \text{ mol O} \times 2 \approx 5 \text{ mol O}$$

Example Empirical Formula Calculation

- An ionic compound used in the brewing industry to clean casks and vats and in the wine industry to kill undesirable yeasts and bacteria is composed of 35.172% potassium, 28.846% sulfur, and 35.982% oxygen. What is the empirical formula for this compound?
- **Step 5:** The resulting mole values correspond to the subscripts in the empirical formula.



Calculating Molecular Formulas



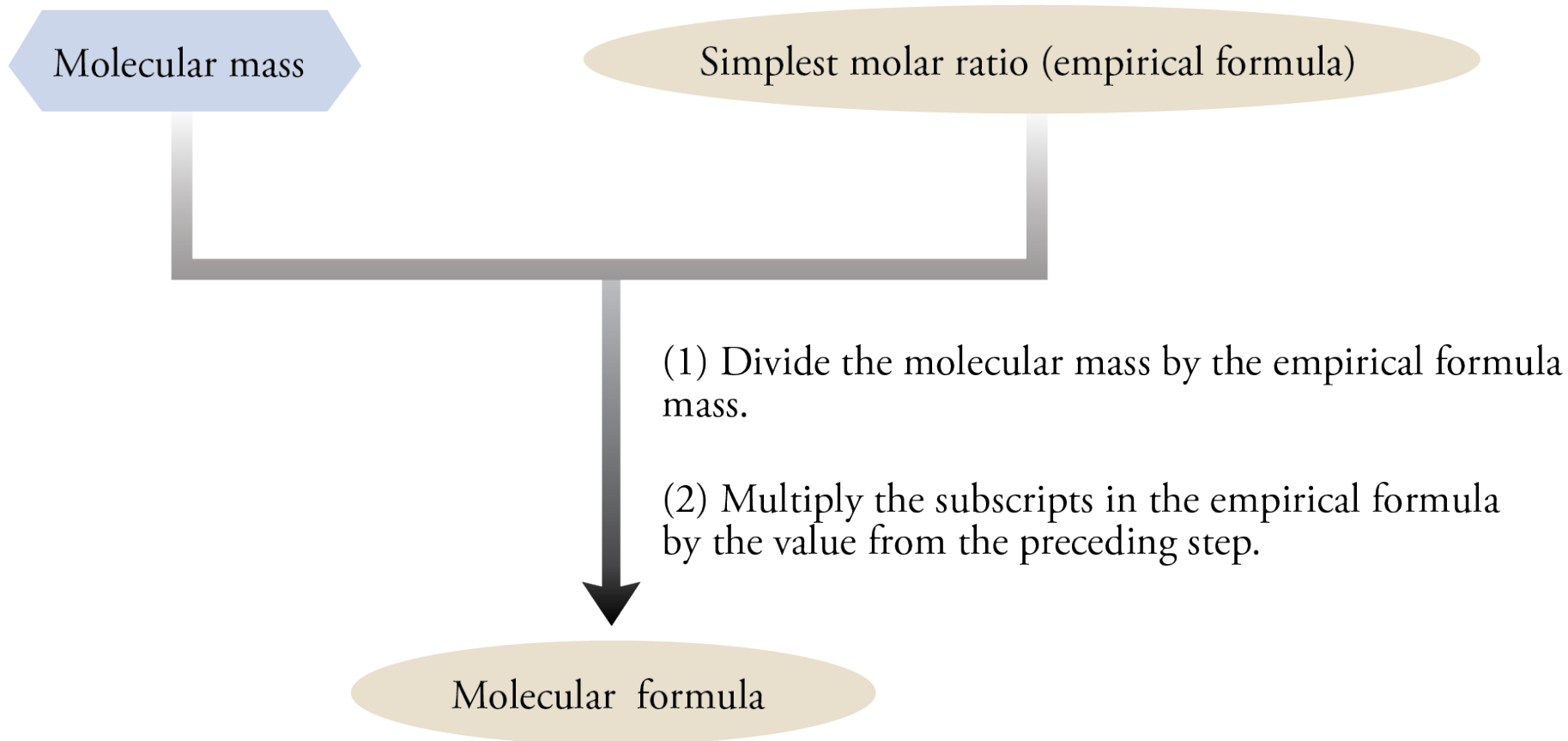
Step 1: If necessary, calculate the empirical formula of the compound from the data given.

Step 2: Divide the given molecular mass by the empirical formula mass.

$$n = \frac{\text{molecular mass}}{\text{empirical formula mass}}$$

Step 3: Multiply each of the subscripts in the empirical formula by n to get the molecular formula.

Calculating Molecular Formulas



Example Molecular Formulas



- Compounds called polychlorinated biphenyls (PCBs) have structures similar to chlorinated insecticides, such as DDT. They have been used in the past for a variety of purposes, but because they have been identified as serious pollutants, their use today is limited to insulating fluids in electrical transformers. They have been banned for even this use in the U.S., but because they and the transformers last a long time, they are still in many transformers, even in the United States. One PCB is 39.94% carbon, 1.12% hydrogen, and 58.94% chlorine and has a molecular mass of 360.88. What is its molecular formula?

Example Molecular Formulas

One PCB is 39.94% carbon, 1.12% hydrogen, and 58.94% chlorine and has a molecular mass of 360.88. What is its molecular formula?

Step 1: If necessary, calculate the empirical formula of the compound from the data given.

$$? \text{ mol C} = 39.94 \text{ g C} \left(\frac{1 \text{ mol C}}{12.011 \text{ g C}} \right) = 3.325 \text{ mol C} \div 1.11 \approx 3 \text{ mol C} \times 2 = 6 \text{ mol C}$$

$$? \text{ mol H} = 1.12 \text{ g H} \left(\frac{1 \text{ mol H}}{1.00794 \text{ g H}} \right) = 1.11 \text{ mol H} \div 1.11 = 1 \text{ mol H} \times 2 = 2 \text{ mol H}$$

$$? \text{ mol Cl} = 58.94 \text{ g Cl} \left(\frac{1 \text{ mol Cl}}{35.4527 \text{ g Cl}} \right) = 1.662 \text{ mol Cl} \div 1.11 = 1\frac{1}{2} \text{ mol Cl} \times 2 = 3 \text{ mol Cl}$$

Empirical formula: $\text{C}_6\text{H}_2\text{Cl}_3$

Example Molecular Formulas

One PCB is 39.94% carbon, 1.12% hydrogen, and 58.94% chlorine and has a molecular mass of 360.88. What is its molecular formula?

Step 2: Divide the given molecular mass by the empirical formula mass.

Step 3: Multiply each of the subscripts in the empirical formula by n to get the molecular formula.

$$\text{Empirical formula: } \text{C}_6\text{H}_2\text{Cl}_3 \quad n = \frac{\text{molecular mass}}{\text{empirical formula mass}} = \frac{360.88}{180.440} \approx 2$$

