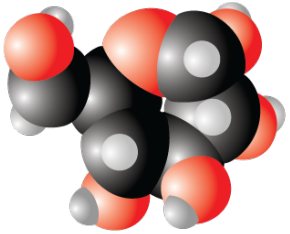
Empirical and Molecular Formulas

- 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 – $C_6H_{12}O_6$
  - Empirical formula – CH_2O

hydrogen peroxide
molecular formula, H_2O_2,
empirical formula, HO



glucose
molecular formula, $C_6H_{12}O_6$,
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

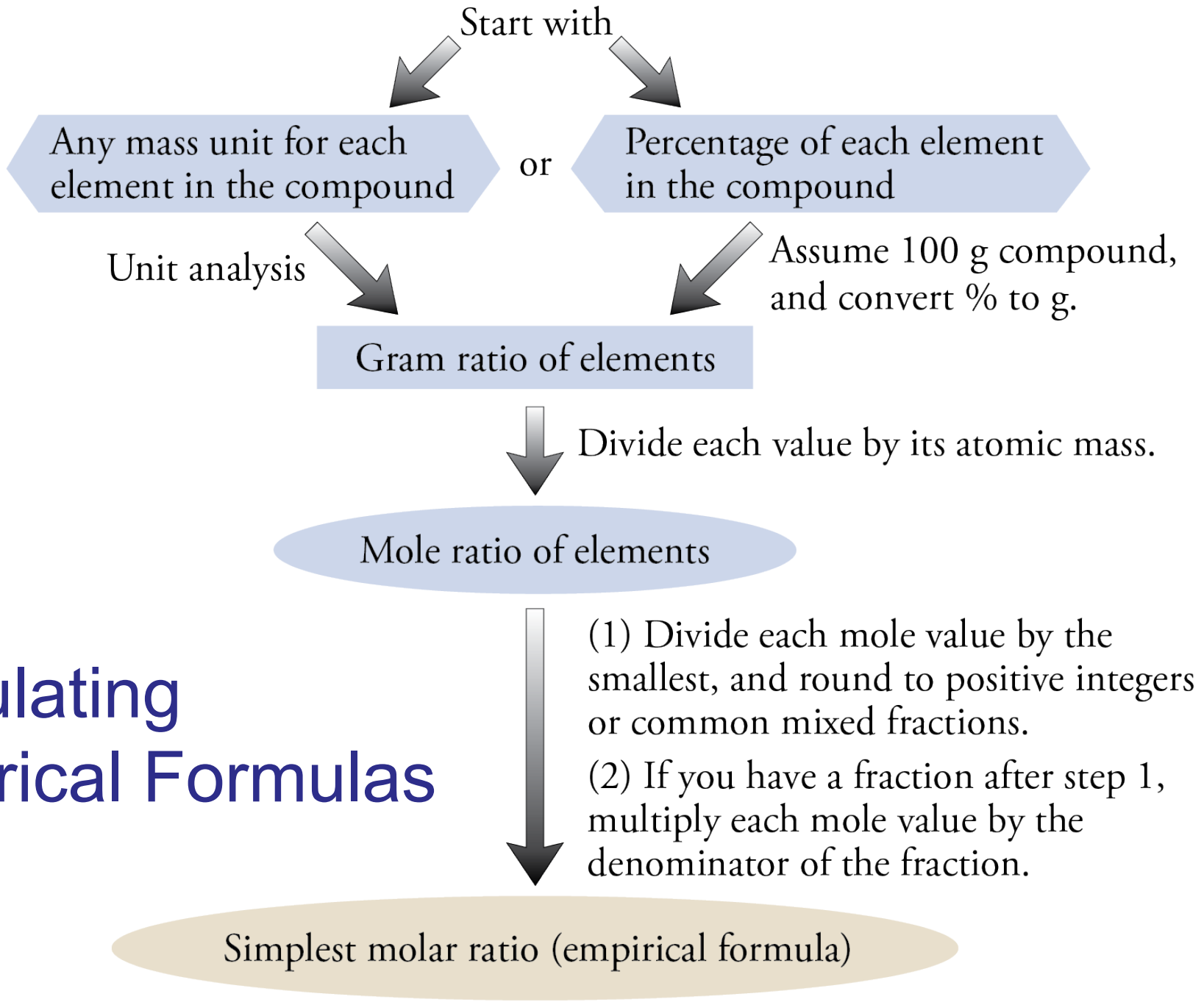
Step 2: Convert grams of each element to moles by dividing by the atomic mass of the element.

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.

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

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

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.

$$K_2S_2O_5$$

Calculating Molecular Formulas

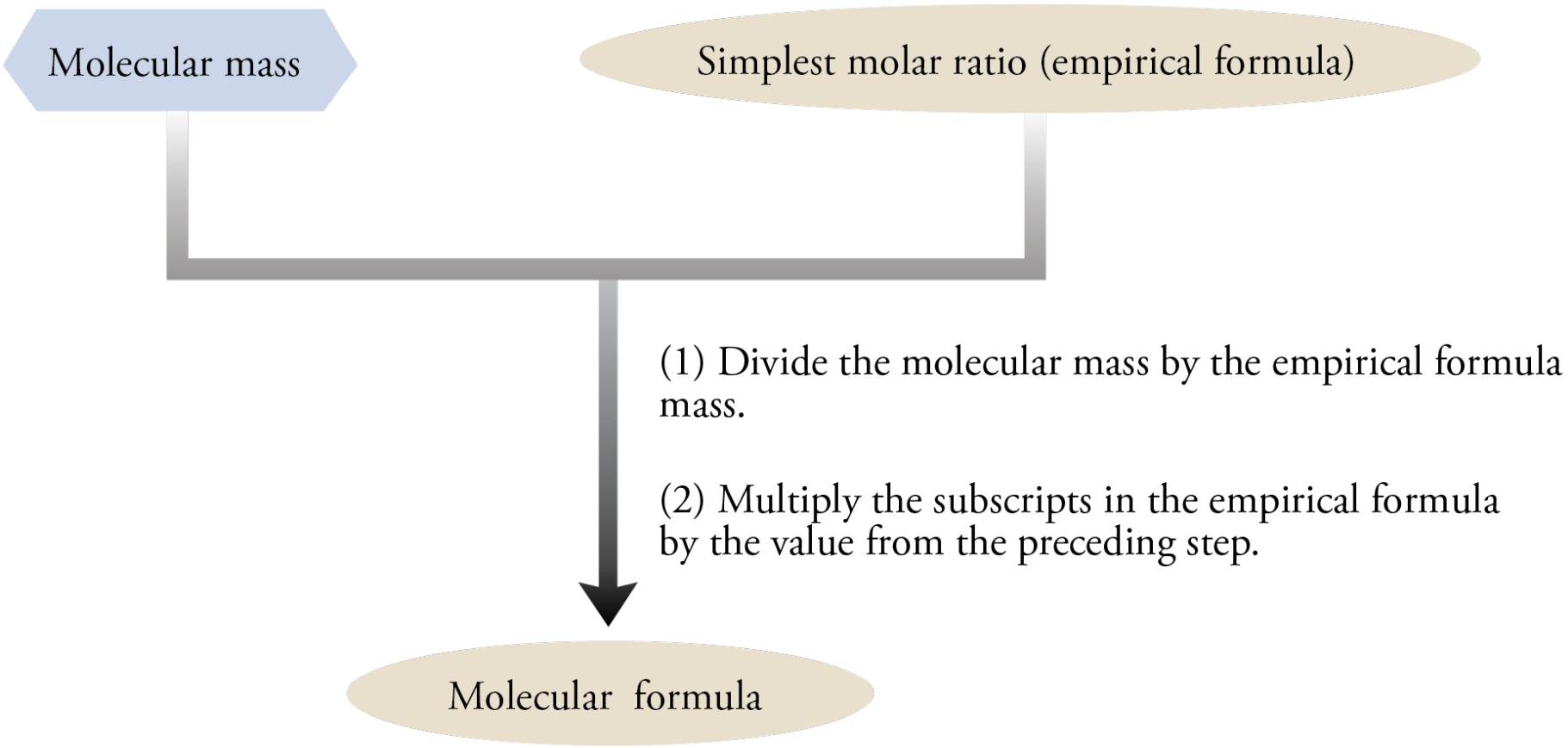
Step 1: If necessary, calculate the empirical formula of the compound from the data given.

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.

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

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

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

Empirical formula: $C_6H_2Cl_3$

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.

Empirical formula: $C_6H_2Cl_3$ $n = \dfrac{\text{molecular mass}}{\text{empirical formula mass}} = \dfrac{360.88}{180.440} \approx 2$

Molecular formula: $\mathbf{C_{12}H_4Cl_6}$