6.6 Empirical and 6.7 Molecular Formulas

Types of Formulas

Two kinds:

1. **Empirical formula**
2. **Molecular(true) formula.**

Empirical	Molecular	Name
CH	C_2H_2	acetylene
CH	C_6H_6	benzene
CO_2	CO_2	carbon dioxide
CH_2O	$C_5H_{10}O_5$	ribose

6.6 Empirical Formulas

Write your own one-sentence definition for each of the following:

Empirical formula

Molecular formula

- **An empirical formula represents the *simplest whole number ratio of the atoms in a compound.***
- **The molecular formula is the *true or actual ratio of the atoms in a compound.***

Learning Check EF-1

A. What is the empirical formula for C_4H_8?

Learning Check EF-2

B. What is a molecular formula for CH_2O?

Learning Check EF-2

If the molecular formula has 4 atoms of N, what is the molecular formula if SN is the empirical formula? Explain.

Determination of Empirical Formulas

What is the empirical formula of a substance that contains Cl, C, and H?

$Cl_X\ C_Y\ H_Z$

What do the X, Y, and Z represent?

Empirical formulas are determined from percent composition experiments

- Elemental analysis that usually involves burning the sample → combustion analysis

Finding the Empirical Formula

The problem:

Combustion analysis showed that a compound is Cl 71.65%, C 24.27%, and H 4.07%. What is the empirical formula?

1. State mass percents as grams in a 100.00-g sample of the compound.

Cl 71.65% ⟶ Cl 71.65 g

C 24.27% ⟶ C 24.27 g

H 4.07% ⟶ H 4.07 g

2. Calculate the number of moles of each element.

$$71.65\text{ g Cl} \times \frac{1\text{ mol Cl}}{35.5\text{ g Cl}} = 2.02\text{ mol Cl}$$

$$24.27\text{ g C} \times \frac{1\text{ mol C}}{12.0\text{ g C}} = 2.02\text{ mol C}$$

$$4.07\text{ g H} \times \frac{1\text{ mol H}}{1.01\text{ g H}} = 4.04\text{ mol H}$$

Why moles?

Why do you need the number of moles of each element in the compound?

Remember what the subscripts in the formula mean.

3. Find the smallest *whole number ratio* by dividing each mole value by the smallest mole value:

Cl: $\frac{2.02}{2.02}$ = 1 Cl

C: $\frac{2.02}{2.02}$ = 1 C

H: $\frac{4.04}{2.02}$ = 2 H

4. Clear decimal by multiplying by an integer

A fraction between 0.1 and 0.9 must not be rounded.

Multiply all results by an integer to give whole numbers for subscripts.

(1/2)	0.5	x 2	=	1
(1/3)	0.333	x 3	=	1
(1/4)	0.25	x 4	=	1
(3/4)	0.75	x 4	=	3

No decimals…..

Cl: $\frac{2.02}{2.02}$ = 1 Cl

C: $\frac{2.02}{2.02}$ = 1 C

H: $\frac{4.04}{2.02}$ = 2 H

5. Write the empirical formula

$Cl_1 C_1 H_2$

ones are understood and not usually written : Cl C H_2

Learning Check

Aspirin is 60.0% C, 4.5 % H and 35.5 O. Calculate its simplest formula.

Remember steps 1, 2, 3, 4, 5:

1. Convert % to g.
2. Calculate moles of each element.
3. Calculate whole mole ratio by dividing by the smallest mole value.
4. Multiply by an integer if needed.
5. Write the formula

Step 1. Convert % to grams

C: 60.0% → 60.0 g

H: 4.5% → 4.5 g

O: 35.5% → 35.5 g

Step 2. Convert grams to moles

$$60.0\text{ g C} \times \frac{1\text{ mol C}}{12.0\text{ g C}} = 5.00\text{ mol C}$$

$$4.5\text{ g H} \times \frac{1\text{ mol H}}{1.01\text{ g H}} = 4.5\text{ mol H}$$

$$35.5\text{ g O} \times \frac{1\text{mol O}}{16.0\text{ g O}} = 2.22\text{ mol O}$$

Step 3. Divide by the smallest # of moles

$$\frac{5.00\text{ mol C}}{2.22\text{ mol O}} = 2.25$$

$$\frac{4.5\text{ mol H}}{2.22\text{ mol O}} = 2.00$$

$$\frac{2.22\text{ mol O}}{2.22\text{ mol O}} = 1.00$$

Are are the results whole numbers? **NO!**

Step 4. Multiply by an integer to clear decimal

Multiply by 4:

C: 2.25 mol C x 4 = 9 mol C

H: 2.0 mol H x 4 = 8 mol H

O: 1.00 mol O x 4 = 4 mol O

Step 5. Write the formula using the whole numbers of mols as the subscripts in the formula

$C_9H_8O_4$

6.6 Types of Formulas

Two kinds:

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2. Molecular(true) formula.

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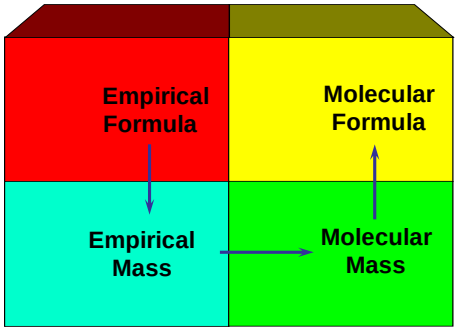
6.7 Molecular Formulas

$$\frac{\text{molar mass}}{\text{simplest mass}} = \text{a whole number} = n$$

n = 1 molar mass = empirical mass
molecular formula = empirical formula

n = 2 molar mass = 2 x empirical mass
molecular formula = 2 x empirical formula

molecular formula = or > empirical formula



Learning Check EF-3

A compound has a formula mass of 176.0 and an empirical formula of $C_3H_4O_3$. What is the molecular formula?

Solution EF-3

A compound has a formula mass of 176.0 and an empirical formula of $C_3H_4O_3$. What is the molecular formula?

$C_3H_4O_3$ = 88.0 g/EF

$\frac{176.0}{88.0} = 2.00$ $\quad (C_3H_4O_3)_{x2} = C_6H_8O_6$

Learning Check EF-4

If there are 192.0 g of O in the molecular formula, what is the true formula if the EF is $C_7H_6O_4$?

Solution EF-4

If there are 192.0 g of O in the molecular formula, what is the true formula if the EF is $C_7H_6O_4$?

EF: 4O x 16 = 64 g O

MF/EF =

$\frac{192 \text{ g O in MF}}{64.0 \text{ g O in EF}} = 3$, therefore

3 x $C_7H_6O_4$ EF = $C_{21}H_{18}O_{12}$ MF