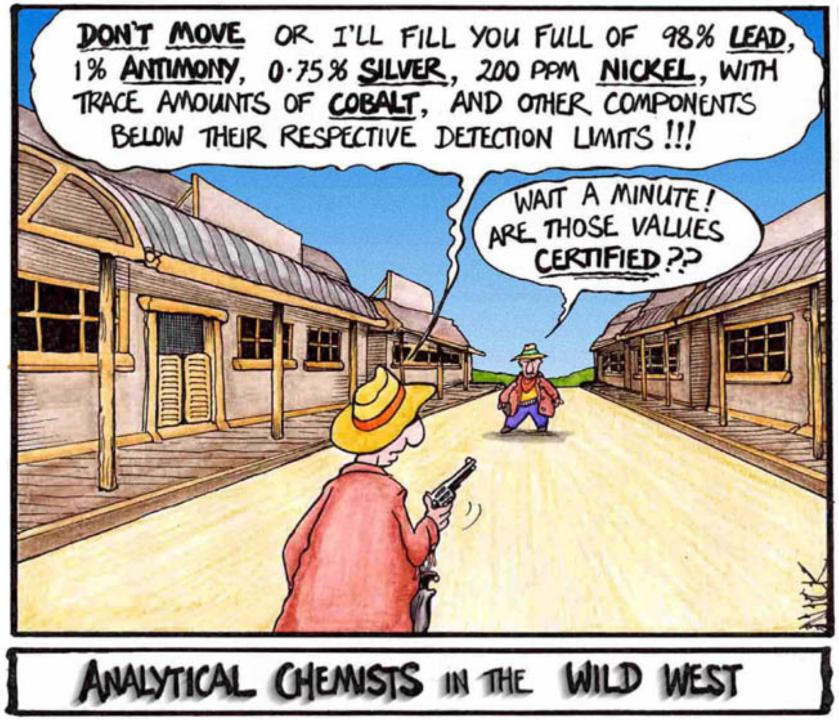
Empirical & Molecular Formulas



Outcome:

Determine empirical and molecular formulas from percent composition or mass data.

Empirical & Molecular Formulas

In a **CHEMICAL FORMULA** the elements are represented by **SYMBOLS**, and a **SUBSCRIPT** number represents the **NUMBER** of each **ELEMENT**.

There are different types:

1. **Molecular Formulae:**
   - Represents the **ACTUAL NUMBER** of atoms of each element **RATHER THAN** a **RATIO** of atoms.
   - The formulas we have been using all along…

Ex) ethane = C_2H_6

PROPANE = C_3H_8

Empirical & Molecular Formulas

2. Empirical Formulae:

- Represents the **RATIOS** of atoms of each element in the compound.
- Is the **REDUCED** or **SIMPLEST** form of the molecular formula

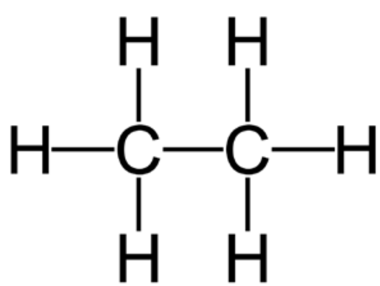
Ex) ethane = CH_3

propane = C_3H_8

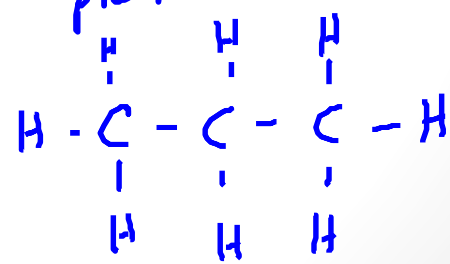
3. Structural Formulae:

- **SHOW** the **BONDS** that connect each atom, and the **STRUCTURE** of the resulting **MOLECULE**.

Ex) ethane:



propane



Empirical & Molecular Formulas

Percent Composition:

- Shows the **PERCENTAGE** of a **COMPOUND`S TOTAL MASS** that each **ELEMENT TAKES** up.
- Can be found from the compound's **FORMULA**, or by **EXPERIMENT**.

$$\frac{Mass_{Element}}{Mass_{Compound}} \bullet 100\%$$

Example:

A 10g sample of propane contains 1.83g of hydrogen. What is the percent composition of propane?

$$\frac{1.83g}{10g} \times 100 = 18.3\%$$

Empirical & Molecular Formulas

Determining Empirical Formulas:

There is a rhyme that we can use to remember the steps…

Percent to mass

Mass to moles

Divide by Small

Times 'till Whole

Empirical & Molecular Formulas

Examples:

1. A compound has a composition of 40.0% carbon, 6.714% hydrogen, and 53.29% oxygen. Determine the empirical formula.

Assume 100g Sample . . .

$$40g\ C \times \frac{1\ mol}{12\ g} = 3.33\ mol\ C \div 3.33 = 1$$

$$6.714\ g\ H \times \frac{1\ mol}{1.01\ g} = 6.65\ mol\ H \div 3.33 = 2$$

$$53.29\ g\ O \times \frac{1\ mol}{16\ g} = 3.33\ mol\ O \div 3.33 = 1$$

$\therefore$ empirical = $C_1H_2O_1$

Empirical & Molecular Formulas

Examples:

2. A compound contains 82.66% carbon atoms and 17.34% hydrogen atoms. Determine the empirical formula

C_xH_y

Assume 100g Sample

$$82.66\text{g C} \times \frac{1\text{ mol}}{12\text{ g}} = \frac{6.89\text{ mol C}}{6.89} = 1 \times 2 = 2$$

$$17.34\text{g H} \times \frac{1\text{ mol}}{1.01\text{ g}} = \frac{17.17\text{ mol H}}{6.89} = 2.5 \times 2 = 5$$

$\therefore$ empirical is C_2H_5

Empirical & Molecular Formulas

Determining Molecular Formulas:

We can use **PERCENT COMPOSITION** and **MOLAR MASS** to determine the molecular formula of a compound.

Example:

A compound contains 71.65% chlorine, 24.27% carbon, and 4.07% hydrogen. Find the **molecular** formula if the molar mass is 98.96 g/mol

Assume 100g Sample

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

$24.27g \times \frac{1mol}{12g} = 2.02 mol\ C \div 2.02 = 1$

$4.07g \times \frac{1mol}{1.01g} = 4.03 mol\ H \div 2.02 = 2$

$\therefore$ empirical = CH_2Cl

↳ mass = 49.52 g/mol

$molecular = \frac{98.96 g/mol}{49.52} = 2 \times$ Bigger

$\therefore$ molecular: $C_2H_4Cl_2$

Empirical & Molecular Formulas

We can also use the relative masses of the elements to determine the formulas…

Example:

If a compound contains 7.3g sodium, 5.08g of sulphur, and 7.63g of oxygen, find the ***simplest*** formula of the compound.

$$7.3\text{g Na} \times \frac{1\text{mol}}{23\text{ g}} = \frac{0.32\text{ mol Na}}{0.16} = 2$$

$$5.08\text{g S} \times \frac{1\text{mol}}{32.1\text{ g}} = \frac{0.16\text{ mol S}}{0.16} = 1$$

$$7.63\text{g O} \times \frac{1\text{mol}}{16\text{ g}} = \frac{0.48\text{ mol O}}{0.16} = 3$$

∴ empirical

Na_2SO_3

Empirical & Molecular Formulas

Try these ones…

1. A compound was analyzed and found to contain 13.5g Ca, 10.8g O, and 0.675g H. What is the empirical formula for the compound?

CaO_2H_2

$$13.5\text{g Ca} \times \frac{1\text{mol}}{40.1\text{g}} = \frac{0.377\text{mol Ca}}{0.377} = 1$$

$$10.8\text{g O} \times \frac{1\text{mol}}{16\text{g}} = \frac{0.675\text{mol O}}{0.377} = 2$$

$$0.675\text{g H} \times \frac{1\text{mol}}{1.01\text{g}} = \frac{0.668\text{mol H}}{0.377} = 2$$

$\therefore CaO_2H_2$

$Ca(OH)_2$

Empirical & Molecular Formulas

Try these ones…

2. NutraSweet is 57.14% C, 6.16% H, 9.52% N, & 27.18% O. Calculate the empirical formula of NutraSweet and find the molecular formula. (The molar mass is 294.30 g/mol) ↳ $C_{14}H_{18}N_2O_5$

Assume 100g Sample . . .

$57.14\,g\,C \times \frac{1\,mol}{12\,g} = \frac{4.76\,mol\,C}{0.68} = 7.0 \times 2 = 14$

$6.16\,g\,H \times \frac{1\,mol}{1.01\,g} = \frac{6.10\,mol\,H}{0.68} = 9 \times 2 = 18$

$9.52\,g\,N \times \frac{1\,mol}{14\,g} = \frac{0.68\,mol\,N}{0.68} = 1 \times 2 = 2$

$27.18\,g\,O \times \frac{1\,mol}{16\,g} = \frac{1.7\,mol\,O}{0.68} = 2.5 \times 2 = 5$

∴ Empirical $= C_{14}H_{18}N_2O_5$

↳ MASS = 294.3 g/mol

∴ Molecular $= C_{14}H_{18}N_2O_5$