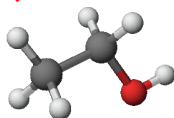


## Law of Definite Proportions

A pure compound always consists of the same elements combined in the same proportions by mass.

Therefore, we can express molecular composition as **percent by mass**

**Ethanol,  $C_2H_6O$**   
**52.13% C**  
**13.15% H**  
**34.72% O**



Syllabus Learning Outcomes : 7

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## Empirical and Molecular Formulas

- A **molecular formula** gives the number of each kind of atom in a molecule.
- An **empirical formula** gives the (whole number) **ratio** of atoms of elements in a compound.

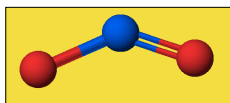
Compound	Molecular formula	Empirical formula
Hydrogen peroxide	$H_2O_2$	HO
Octane	$C_8H_{18}$	????

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## Percent Composition

Consider some of the family of nitrogen-oxygen compounds:

$NO_2$ , nitrogen dioxide and closely related, NO, nitrogen monoxide (or nitric oxide)



Structure of  $NO_2$

Chemistry of NO,  
nitrogen monoxide



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## Calculate Mass Percent Composition

Consider  $NO_2$ , Molar mass = ?

What is the mass percent of N and of O?

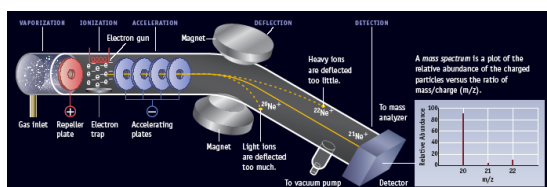
$$\text{Mass \% N} = \frac{14.0 \text{ g N}}{46.0 \text{ g } NO_2} \cdot 100\% = 30.4\%$$

$$\text{Mass \% O} = \frac{2(16.0 \text{ g O})}{46.0 \text{ g } NO_2} \cdot 100\% = 69.6\%$$

What are the mass percentages of N and O in NO?

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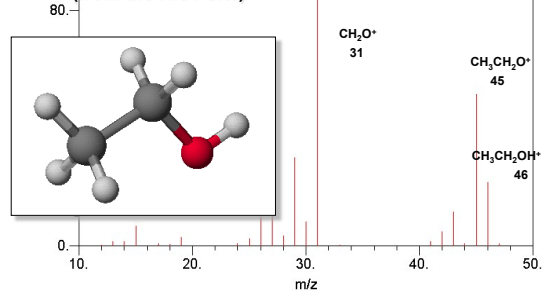
## How to Determine a Formula?



Mass spectrometer

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Mass Spectrum of Ethanol  
(from the NIST site)



## Determining Formulas

In **chemical analysis** we determine the % by mass of each element in a given amount of pure compound and derive the **EMPIRICAL** or **SIMPLEST** formula.

**PROBLEM:** A compound of B and H is 81.10% B. What is its empirical formula?



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A compound of B and H is 81.10% B. What is its empirical formula?

- Because it contains only B and H, it must contain 18.90% H.
- In 100.0 g of the compound there are 81.10 g of B and 18.90 g of H.
- Calculate the number of moles of each constituent.

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A compound of B and H is 81.10% B. What is its empirical formula?

Calculate the number of moles of each element in 100.0 g of sample.

$$81.10 \text{ g B} \cdot \frac{1 \text{ mol}}{10.81 \text{ g}} = 7.502 \text{ mol B}$$

$$18.90 \text{ g H} \cdot \frac{1 \text{ mol}}{1.008 \text{ g}} = 18.75 \text{ mol H}$$

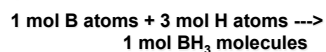
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A compound of B and H is 81.10% B. What is its empirical formula?

Now, recognize that **atoms combine in the ratio of small whole numbers.**



or



Find the ratio of moles of elements in the compound.

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A compound of B and H is 81.10% B. What is its empirical formula?

Take the ratio of moles of B and H. **Always divide by the smaller number.**

$$\frac{18.75 \text{ mol H}}{7.502 \text{ mol B}} = \frac{2.499 \text{ mol H}}{1.000 \text{ mol B}} = \frac{2.5 \text{ mol H}}{1.0 \text{ mol B}}$$

But we need a whole number ratio.

$$2.5 \text{ mol H} / 1.0 \text{ mol B} = 5 \text{ mol H to 2 mol B}$$

**EMPIRICAL FORMULA = B<sub>2</sub>H<sub>5</sub>**

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## Determining Formulas - Recap

**PROBLEM:** A compound of B and H is 81.10% B. What is its empirical formula?

• Stepwise solution

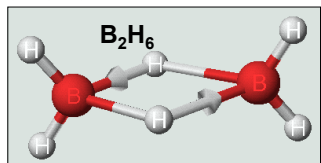


- B 81.10% 81.10g 7.502mol 1 2 B<sub>2</sub>H<sub>5</sub>
- H 18.90% 18.90g 18.75mol 2.5 5

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A compound of B and H is 81.10% B. Its empirical formula is  $B_2H_5$ . What is its molecular formula?

Is the molecular formula  $B_2H_5$ ,  $B_4H_{10}$ ,  $B_6H_{15}$ ,  $B_8H_{20}$ , etc.?



$B_2H_6$  is one example of this class of compounds.

B = 10.811  
H = 1.0079

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A compound of B and H is 81.10% B. Its empirical formula is  $B_2H_5$ . What is its molecular formula?

We need to do an **EXPERIMENT** to find the MOLAR MASS.

Here experiment gives **53.3 g/mol**

Compare with the mass of  $B_2H_5$

= **26.66 g/unit**

B = 10.811  
H = 1.0079

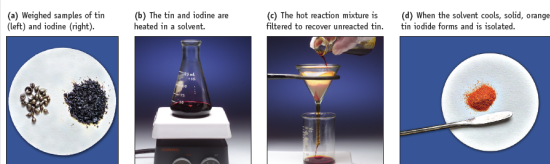
Find the ratio of these masses.

$$\frac{53.3 \text{ g/mol}}{26.66 \text{ g/unit of } B_2H_5} = \frac{2 \text{ units of } B_2H_5}{1 \text{ mol}}$$

**Molecular formula =  $B_4H_{10}$**

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### DETERMINE THE FORMULA OF A COMPOUND OF Sn AND I



Have g of Sn used, (excess)      g of  $I_2$  used,      and g of  $SnI_x$  formed

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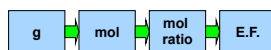
### Data to Determine the formula of a Sn—I Compound

- Reaction of Sn and  $I_2$  is done using excess Sn.
- Mass of Sn in the beginning = 1.056 g
- Mass of iodine ( $I_2$ ) used = 1.947 g
- Mass of Sn remaining = 0.601 g

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### Determining Formulas

- Similar stepwise solution



Sn

$I_2$

- Watch how much Sn used, how much I

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### Tin and Iodine Compound

Find the mass of Sn that combined with 1.947 g  $I_2$ .

Mass of Sn initially = 1.056 g

Mass of Sn recovered = 0.601 g

Mass of Sn used = 0.455 g

Find moles of Sn used:

$$0.455 \text{ g Sn} \cdot \frac{1 \text{ mol}}{118.7 \text{ g}} = 3.83 \times 10^{-3} \text{ mol Sn}$$

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### Tin and Iodine Compound

Now find the number of moles of  $I_2$  that combined with  $3.83 \times 10^{-3}$  mol Sn. Mass of  $I_2$  used was 1.947 g.

$$1.947 \text{ g } I_2 \cdot \frac{1 \text{ mol}}{253.81 \text{ g}} = 7.671 \times 10^{-3} \text{ mol } I_2$$

How many mol of **iodine atoms**?

$$7.671 \times 10^{-3} \text{ mol } I_2 \left( \frac{2 \text{ mol I atoms}}{1 \text{ mol } I_2} \right)$$

$$= 1.534 \times 10^{-2} \text{ mol I atoms}$$

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### Tin and Iodine Compound

Now find the ratio of number of moles of moles of I and Sn that combined.

$$\frac{1.534 \times 10^{-2} \text{ mol I}}{3.83 \times 10^{-3} \text{ mol Sn}} = \frac{4.01 \text{ mol I}}{1.00 \text{ mol Sn}}$$

Empirical formula is **SnI<sub>4</sub>**

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### Determining Formulas of Hydrated Compounds

- Similar solution approach to other problems

- In the lab, heat hydrated copper sulfate and collect these data:



- What is x for the number of moles of water?

Need mass of water first, g

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### Determine Mass of Water

Mass of hydrated compound	1.023 g
Mass of anhydrous compound	<u>- 0.654 g</u>
Mass of water	0.369 g

Solution is just like for determining empirical formulas (g to mol to mol ratio to simplest whole number ratio to formula)

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### Calculate Moles

$$0.369 \text{ g H}_2\text{O} \cdot \frac{1 \text{ mol H}_2\text{O}}{18.02 \text{ g H}_2\text{O}} = 0.0205 \text{ mol H}_2\text{O}$$

$$0.654 \text{ g CuSO}_4 \cdot \frac{1 \text{ mol CuSO}_4}{159.6 \text{ g CuSO}_4} = 0.00410 \text{ mol CuSO}_4$$

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### Determine Mole Ratios and Empirical Formula

- Find simplest whole number mole ratio

$$\frac{0.0205 \text{ mol H}_2\text{O}}{0.00410 \text{ CuSO}_4} = \frac{5 \text{ mol H}_2\text{O}}{1 \text{ mol CuSO}_4}$$

- Write the empirical formula



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### Summary

- Determine the **mass percent** or **percent composition** of each element of a molecule using the **molecular formula**
- Determine an **empirical formula** using **percent composition** (%  $\rightarrow$  g  $\rightarrow$  mol  $\rightarrow$  mol ratios).
- Determine a molecular formula using molar mass or molecular weight.