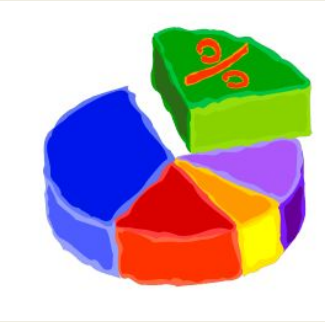
DETERMINING CHEMICAL FORMULAS

Percent Composition

- Percentage composition: the percentage by mass of each element in a compound
  - Describes the chemical composition of a compound
- *The percentage of an element in a compound is the same regardless of the sample's size*



- **How to determine the percent composition of a compound**:
  1. Find the mass of each element in the compound
  2. Find the total mass of the compound
  3. Determine the percent composition of each element in the compound

Sample Problem

Find the percentage composition of copper(I) sulfide, Cu_2S.

- Given: formula, Cu_2S
- Unknown: percent composition of Cu_2S
- Solve:

1. Find the mass of each element in the compound

   2 mol Cu x (63.55 g/mol Cu) = 127.1 g Cu

   1 mol S x (32.07 g/mol S) = 32.07 g S

2. Find the total mass of the compound

   Total mass of Cu_2S = 127.1 g + 32.07 g = 159.2 g Cu_2S

3. Determine the percent composition of each element in the compound

$$\frac{127.1\text{ g Cu}}{159.2\text{ g } Cu_2S} \times 100 = 79.84\ \%\ \text{Cu} \qquad \frac{32.07\text{ g S}}{159.2\text{ g } Cu_2S} \times 100 = 20.14\ \%\ \text{S}$$

You Try!

Find the percent composition of the following compounds:

- **Lead(II) chloride, $PbCl_2$**
  - 74.51% Pb
  - 25.49% Cl
- **Barium nitrate, $Ba(NO_3)_2$**
  - 52.55% Ba
  - 10.72% N
  - 36.73% O

- Calculate the percent composition of HgO.
  - Hg = 92.6% ; O = 7.40 %
- Determine the percent composition of lithium bromide.
  - Li = 7.99% ; Br = 92.0%

Empirical Formula

- Empirical formula: consists of the symbols for the elements combined in a compound, with subscripts showing the *smallest whole-number mole ratio* for the different atoms in the compound
  - For an ionic compound: the formula unit is usually the compound's empirical formula
  - For a molecular compound: the empirical formula does not necessarily indicate the actual numbers of atoms present in each molecule

MOLECULAR	EMPIRICAL
P_4O_{10}	P_2O_5
$C_{10}H_{22}$	C_5H_{11}
$C_6H_{18}O_3$	C_3H_6O
$C_5H_{12}O$	$C_5H_{12}O$
N_2O_4	NO_2

How to Calculate Empirical Formulas

Percentage composition → Mass composition → Mole composition → Smallest whole-number mole ratio of atoms

1. If necessary, begin by converting percentage composition to a mass composition
   - Assume that you have 100.0 g of sample of the compound
2. Determine the amount in moles of each element by dividing the appropriate molar mass
3. Determine the smallest value from Step 2
4. Divide all moles by the smallest number in the existing ratio
   - Round each number to the nearest whole number
5. Use the whole numbers from Step 4 as subscripts

Sample Problem

Quantitative analysis shows that a compound contains 32.38% sodium, 22.65% sulfur, and 44.99% oxygen. Find the empirical formula of this compound.

- Given: Percent composition Unknown: Empirical formula
- Solve:
  1. *Mass composition*:

     32.38 g Na; 22.65 g S; 44.99 g O

  2. *Composition in moles*:

$$\frac{32.38\text{ g Na}}{22.99\text{ g/mol Na}} = 1.408\text{ mol Na} \qquad \frac{22.65\text{ g S}}{32.07\text{ g/mol S}} = 0.706\text{ mol S}$$

$$\frac{44.99\text{ g O}}{16.00\text{ g/mol O}} = 2.812\text{ mol O}$$

3. *Smallest value from Step 2*:

   0.706 mol

4. *Smallest whole-number ratio*:

$$\frac{1.408 \text{ mol}}{0.706 \text{ mol}}\ \text{Na} : \frac{0.706 \text{ mol}}{0.706 \text{ mol}}\ \text{S} : \frac{2.812 \text{ mol}}{0.706 \text{ mol}}\ \text{O}$$

$$= 1.993 \text{ mol Na} : 1.00 \text{ mol S} : 3.981 \text{ mol O}$$

$$= 2 \text{ mol Na} : 1 \text{ mol S} : 4 \text{ mol O}$$

3. *Use whole-numbers from Step 4 as subscripts*:

   $Na_2S_1O_4$ Empirical formula = Na_2SO_4

You Try!

- A compound is found to contain 63.42% iron and 36.48% sulfur. Find its empirical formula.
  - FeS
- Determine the empirical formula of the compound that contains 17.15% carbon, 1.44% hydrogen, and 81.41% fluorine.
  - CHF_3

Another Empirical Formula Sample Problem

A compound is found to contain only phosphorus and oxygen. There are 4.433 g of phosphorus and 5.717 g of oxygen found in the compound. What is the compound's empirical formula?

- Given: 4.433 g P ; 5.717 g O Unknown: Empirical formula
- Solve:
  - *Mass composition*: 4.433 g P ; 5.717 g O
  - *Mole composition*:
    - $\frac{4.433\text{ g P}}{30.97\text{ g/mol P}} = 0.1431\text{ mol P}$ $\frac{5.717\text{ g O}}{16.00\text{ g/mol O}} = 0.3573\text{ mol O}$
  - *Smallest whole-number ratio*:
    - $\frac{0.1431}{0.1431} = 1\text{ mol P}$ $\frac{0.3573}{0.1431} = 2.497\text{ mol O}$

How would you round 2.5 though?

If the mole ratio ends in a 0.5, *Multiply everything by 2*!

- So…
  - $\frac{0.1431}{0.1431}$ = 1 mol P $\frac{0.3573}{0.1431}$ = 2.497 mol O
  - becomes…

    1 mol P x 2 2.5 mol O x 2

    = 2 mol P 5 mol O
  - *Use whole numbers as subscripts*:

    Empirical formula = P_2O_5

You Try!

- A sample of an unidentified compound contains 29.84 g sodium, 67.49 g chromium, and 72.67 g oxygen. What is the compound's empirical formula?
  - $Na_2Cr_2O_7$
- Analysis of a compound containing only calcium and bromine indicates that 4.0 g of calcium and 16 g of bromine are present. What is the compound's empirical formula?
  - $CaBr_2$

Calculation of Molecular Formulas

- Relationship between a compound's empirical formula & it's molecular formula can be written as follows:
  - x (empirical formula) = molecular formula
    - *x = whole-number multiple*

- To determine the molecular formula of a compound, you must know the compound's empirical formula and formula mass!
  - *To find x*:

$$x = \frac{\text{experimental formula mass (given mass)}}{\text{empirical formula mass}}$$

Round to the nearest whole number!

Sample Problem

The empirical formula of a compound of phosphorus and oxygen was found to be P_2O_5. Experimentation shows that the molar mass of this compound is 283.89 g/mol. What is the compound's molecular formula?

- Given:
  - Empirical formula: P_2O_5 Molar mass mass = 283.89 g/mol
- Unknown:
  - Molecular formula
- Solve:
  1. *Find the formula mass of the compound.*
     - Recall that formula mass & molar mass are numerically equal
       - Molar mass = 283.89 g/mol
       - Formula mass = 283.89 amu

2. *Find the formula mass of the empirical formula*.

   Empirical formula = P_2O_5

   P = 31.0 amu O = 16.0 amu

   P_2O_5 mass = (2 x 31.0 amu) + (5 x 16.0 amu)

   = 142 amu

3. *Find the x factor by dividing the experimental formula mass (given mass) by the empirical formula mass*.

   $x = \frac{283.89 \text{ amu}}{142 \text{ amu}} = 1.99$ ← *Round to the nearest whole number!*

   = 2

4. Multiply the empirical formula by the x factor to get the molecular formula.

   molecular formula = x (empirical formula)

   = 2 (P_2O_5)

   = P_4O_{10}

You Try!

- Determine the molecular formula of a compound with the empirical formula of CH and a formula mass of 78.11 amu.
  - C_6H_6
- A sample of a compound with a formula mass of 34 amu is found to consist of 0.44 g H and 6.92 g O. Find its molecular formula.
  - H_2O_2