Finding Formulas

using mass information about a compound to find its formula

Molecular Formula

- Molecular formula is the actual formula of compounds which form molecules.
- For example, the molecular formula of water is H_2O, the molecular formula of benzene is C_6H_6.
- This formula represents the ratio of atoms in one molecule of that substance – or moles of each element in one mole of that substance.

Empirical Formula

- Empirical formula is the formula which represents the simplest whole number ratio of the elements in a compound
- For example: a compound with a molecular formula of C_6H_6 has an empirical formula of CH.
- What is the empirical formula of a compound with the molecular formula C_8H_{18}?

Empirical Formula

- To find empirical formula, first convert masses of elements in a compound to moles
- Next calculate the ratio of moles of the elements in the compound
- This ratio will give you the subscripts of the empirical formula

Finding Empirical Formula

Often you will be finding an empirical formula based on mass percent values of a compound.

<u>Sample Problem</u>:

Find the empirical formula of a compound which is 82.22% nitrogen and 17.78% hydrogen by mass.

Finding Empirical Formula

1. Change the percent composition to mass by assuming that you have a 100 gram sample.
2. Convert the masses of the elements into moles of those elements.
3. Divide all of the mole values by the smallest value.
4. Write the formula of the compound using those quotients as the subscripts.

Finding Empirical Formula

1. Change the percent composition to mass by assuming that you have a 100 gram sample.

82.22% Nitrogen 17.78% Hydrogen

82.22 g Nitrogen 17.78 g Hydrogen

Finding Empirical Formula

2. Convert the masses of the elements into moles of those elements.

82.22g N / 14.01 g/mole = 5.87 moles N

17.78g H / 1.01 g/mole = 17.6 moles H

Finding Empirical Formula

3. Divide all of the mole values by the smallest value. This will usually give you a whole number ratio of the moles.

5.87 moles N / 5.87 = 1 moles N

17.6 moles H / 5.87 = 3 moles H

Finding Empirical Formula

4. Write the formula of the compound using those whole numbers as the subscripts.

Subscript for Nitrogen = 1

Subscript for Hydrogen = 3

Empirical Formula = NH_3

Finding Empirical Formula

Of course, some variations are possible.

Instead of % composition, you might be given the masses of the elements found in the compound.

<u>Sample Problem 2</u>:

Find the empirical formula of a compound if a 5.000 g sample contains 2.687 grams of iron and 2.313 grams of sulfur.

Finding Empirical Formula

1. Change the % composition to mass by assuming that you have a 100 gram sample.

In this problem, there is no need to convert the percents to mass. Move on to step 2.

2. Convert the masses of the elements into moles of those elements.

2.687g Fe / 55.85 g/mole = .0481 moles Fe

2.313g S / 32.07 g/mole = .0721 moles S

Finding Empirical Formula

3. Divide all of the mole values by the smallest value.

.0481 moles Fe / .0481 = 1 mole Fe

.0721 moles S / .0481 = 1.5 moles S

Since subscripts of a formula must be whole numbers, you must change these values into whole numbers (get rid of decimals) while keeping the same ratio

To do this, multiply them by 2

1 mole Fe x 2 = 2 moles Fe

1.5 moles S x 2 = 3 moles S

Finding Empirical Formula

4. Write the formula of the compound using those whole numbers as the subscripts.

Subscript for Fe = 2

Subscript for S = 3

Empirical formula = Fe_2S_3

Finding Empirical Formula

1. If given % composition, assume 100 gram sample. If given masses of elements in the compound, move on to step 2.
2. Convert the masses of the elements into moles of those elements.
3. Divide all of the mole values by the smallest mole value. Convert to whole numbers if necessary
4. Write the formula of the compound using those whole numbers as the subscripts.

Finding Empirical Formula

<u>Sample Problem 3</u>:

Find the empirical formula of a compound if a sample contains 7.00 grams of carbon, 1.17 grams of hydrogen, and 9.33 grams of oxygen.

Finding Empirical Formula

7.00 g C / 12.01 g/mole = .583 moles C

1.17 g H / 1.01 g/mole = 1.16 moles H

9.33 g O / 16.00 g/mole = .583 moles

.583 moles C / .583 = 1 mole C

1.16 moles H / .583 = 2 moles H

.583 moles O / .583 = 1 mole O

Empirical Formula = CH_2O

Molecular Formula

- Ionic compounds are usually written with the simplest ratio = empirical formula

- Covalent compounds often have molecular formulas which are whole number multiples of the empirical formula.

Molecular Formula

- To find the molecular formula, you must know the empirical formula and the molar mass of the compound.

- Since the molecular formula is a multiple of the empirical formula, the molar mass is a multiple of the empirical mass.

Finding Molecular Formula

<u>Sample Problem 4</u>:

Find the molecular formula of a compound which contains 7.00 grams of carbon, 1.17 grams of hydrogen, and 9.33 grams of oxygen. The molar mass of this compound is 180.18 g/mole.

Finding Molecular Formula

1. Find the empirical formula of the compound
2. Calculate the empirical mass
3. Divide the molar mass by the empirical mass = whole number
4. Multiply the empirical formula by the number from Step 3 to get molecular formula
5. Check to make sure the molar mass matches what is given in the problem

Finding Molecular Formula

1. Find the empirical formula

We have already found the empirical formula to be CH_2O

2. Calculate the empirical mass – this is the molar mass of the empirical formula

Empirical mass = (1 x 12.01) + (2 x 1.01)
+ (1 x 16.00)

= 30.03 g/mole

Finding Molecular Formula

3. Divide the molar mass by the empirical mass = whole #

180.18 g/mole / 30.03 g/mole = 6

4. Multiply the empirical formula by this number

$(CH_2O) \times 6 = C_6H_{12}O_6$

Finding Molecular Formula

5. Check your work. Make sure that the molar mass of your formula matches the molar mass given in the problem.

$$C_6H_{12}O_6$$

Molar mass = (6 x 12.01) + (12 x 1.01) + (6 x 16.00)

= 180.18 g/mole

This matches the molar mass given

Finding Molecular Formula

<u>Sample Problem #5</u>

Butylene is a hydrocarbon that has a molar mass between 55 and 58 grams per mole. Analysis of butylene reveals that it is 85.60% carbon and 14.40% hydrogen by mass. Find the molecular formula of butylene.

Finding Molecular Formula

1. Find empirical formula

85.60% C = 85.60 g C/12.01 g/mol = 7.127 moles C

14.40% H = 14.40 g H/1.01 g/mol = 14.26 moles H

7.127/7.127 = 1 14.26/7.127 = 2 E.F. = CH_2

2. Calculate the empirical mass

(1 x 12.01) + (2 x 1.01) = 14.03 g/mol

Finding Molecular Formula

3. Divide molar mass by the empirical mass = whole number

In this problem we have a range for molar mass (55 – 58 g/mol) so we need to figure out how many times to multiply the empirical mass to get it into this range.

55/14.03 = 3.92 58/14.03 = 4.13

The multiplier is 4

Finding Molecular Formula

4. Multiply the empirical formula by the whole number from step #3.

$$CH_2 \times 4 = C_4H_8$$

5. Check your answer.

$$(4 \times 12.01) + (8 \times 1.01) = 56.12 \text{ g/mol}$$

This is within the range given in the problem