Percent Composition

One way to identify an unknown compound is to determine the relative mass of the different elements in its make-up — its percent composition by mass. We can use the ideas of moles and molar mass to identify the compound. Before we look at that, it's useful to see how a percent composition is calculated for a known compound.

FINDING PERCENT COMPOSITION

A **percent composition** is a breakdown of how much of the mass of any sample of a compound comes from each element in the compound.

Example 1: What is the percent composition by mass of water?

Solution: Water is H_2O. To find percent composition, we'll need the molar mass of the compound:

$$\begin{aligned} 2 \times H = 2 \times 1.01\ \text{g/mol} &= 2.02 \\ 1 \times O = 16.00\ \text{g/mol} &= \underline{16.00} \\ &= 18.02\ \text{g/mol} \end{aligned}$$

Now we divide this by the mass that each element contributed to the total mass. If an element contributes more than one atom to the molecule, use the mass of the total number of atoms for the element, not just one.

$$\text{H: } 2.02 \div 18.02 = 0.11209\ldots \approx 11.2\%$$
$$\text{O: } 16.00 \div 18.02 = 0.88790\ldots \approx 88.8\%$$

So water is 11.2% hydrogen and 88.8% oxygen by mass.

EMPIRICAL FORMULAS

An **empirical formula** for a compound is a formula that tells you the ratio of atoms of the elements within it (the **molar ratio**), but not the exact number of atoms of each element in the molecule. What's the difference?

Consider NO_2, nitrogen dioxide, which is produced in car exhaust, and N_2O_4, dinitrogen tetroxide, a component of rocket fuel. If I have a sample of each of them, then I know in both cases there are twice as many oxygen atoms in the sample as nitrogen atoms. They're arranged into molecules in different ways, but the proportion of nitrogen to oxygen atoms is still 1 : 2. Both compounds have an empirical formula of NO_2, even though they're completely different chemicals.

If we only know how much of a compound is nitrogen or oxygen by mass, it would be impossible to tell the two apart, but determining the empirical formula of a compound is still the important first step in this kind of analysis.

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Example 2: Determine the empirical formula of a compound that is 60.04% silicon and 39.96% nitrogen by mass.

Solution: We start by assuming that we have 100 grams of this compound. (We're working with a ratio, so any mass will work, and 100 g makes calculations very easy.) Then we figure out how many grams of silicon and oxygen would be in a 100-g sample. Last, we calculate how many moles of these elements are in it using their molar masses.

$$60.04\% \text{ of } 100\text{ g} = 60.04\text{ g of Si} \qquad 60.04\text{ g Si} \times \frac{1\text{ mol Si}}{28.06\text{ g Si}} = 2.1397\ldots\text{ mol Si}$$

$$39.96\% \text{ of } 100\text{ g} = 39.96\text{ g of N} \qquad 39.96\text{ g N} \times \frac{1\text{ mol N}}{14.01\text{ g N}} = 2.8522\ldots\text{ mol N}$$

We still need to determine the ratio between the two. Divide each molar quantity by the smallest one you get. If a decimal results, hopefully you'll recognize it as a fraction. (If not, try dividing it the other way.)

$$2.8522 \div 2.1397 = 1.3330\ldots \approx 1\tfrac{1}{3} = \tfrac{4}{3}$$

If we divided them the other way, we get 0.7502, which is pretty close to $\frac{3}{4}$. Either way, we recognize that the ratio is 3 Si : 4 N, so the empirical formula is Si_3N_4.

We don't know what this compound is exactly, yet. It could be Si_3N_4, or possibly something more complicated like Si_6N_8 or Si_9N_{12}…. We need more information to know for sure. A molar mass for the compound is (relatively) easy to measure and allows us to narrow the field down to one formula. A formula that says explicitly how many atoms of each element are in a compound is called a **molecular formula**.

Example 3: (a) Determine the empirical formula of a compound that is 47.76% oxygen, 34.31% sodium and 17.93% carbon by mass. (b) Determine its molecular formula if its molar mass is 134.002 $^{g}/_{mol}$.

Solution: (a) Assume we have 100 g of this compound.

$$47.76\% \text{ of } 100\text{ g} = 47.76\text{ g of O} \qquad 47.76\text{ g} \times \frac{1\text{ mol O}}{16.00\text{ g O}} = 2.985\text{ mol O}$$

$$34.31\% \text{ of } 100\text{ g} = 34.31\text{ g of Na} \qquad 34.31\text{ g} \times \frac{1\text{ mol Na}}{22.99\text{ g Na}} = 1.4923\ldots\text{ mol Na}$$

$$17.93\% \text{ of } 100\text{ g} = 17.93\text{ g of C} \qquad 17.93\text{ g} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 1.4929\ldots\text{ mol C}$$

We divide: 2.985 ÷ 1.4923 ≈ 2, and 1.4929 ÷ 1.4923 ≈ 1. This means there are 2 oxygen atoms and one carbon atom for every sodium atom, so the empirical formula is O_2NaC, or, putting the metal first and the non-metals in alphabetical order, $NaCO_2$.

(b) Now we have the molar mass. We can easily find out what the actual molecular formula is by dividing the molar mass of the empirical formula by the actual molar mass.

$$\text{Na} + \text{C} + 2(\text{O}) = 22.99 + 12.01 + 2 \times 16.00 = 67.00\ ^{g}/_{mol}$$

$$134.002\ ^{g}/_{mol} \div 67.00 \approx 2$$

This means the actual molecular formula is double the empirical formula: $Na_2C_2O_4$.

Example 4: A chemical with composition AB_2C (where A, B and C are unknown elements) has a percent composition of 51.79% A, 46.74% B and 1.47% C, and a molecular mass of 68.460 g/mol. Identify the compound.

Solution: In this case, we don't know the identities of the elements, so we can't use the same method to solve. We can use the percentages and molecular mass to get a molar ratio more directly. This time, we assume that we have 1 mole of compound, expressed as a mass. The subscript in the formula we've been given for the compound tells us that there are two atoms of Element B, and one each for A and C. We divide by the number of atoms of each element that we know are in the compound. This should give us the molar masses of the elements.

Assume we have 68.460 g of the unknown compound.

A: 51.79% of 68.460 g = 35.45 g	35.45 g ÷ 1 = 35.45 g
B: 46.74% of 68.460 g = 32.00 g	32.00 g ÷ 2 = 16.00 g
C: 1.47% of 68.460 g = 1.01 g	1.01 g ÷ 1 = 1.01 g

When we look at the periodic table, we see that Element A should be chlorine, Element B should be oxygen and element C should be hydrogen. That makes the compound $C\ell O_2H$, or, putting the positive hydrogen first and the negative oxyanion last, $HC\ell O_2$.

EXERCISES

A. Determine the percent composition of these compounds by mass. Round your percentages to one decimal place.

1) quartz, SiO_2
2) methane, CH_4
3) potassium cyanide, KCN
4) ozone, O_3
5) ammonium sulphide, $(NH_4)_2S$
6) caffeine, $C_8H_{10}N_4O_2$

B. 1) Would you get a different percent composition for steam than we did in Example 1 for water? Explain.

2) Would the percent composition for hydrogen peroxide, H_2O_2, be different than for water? Explain.

3) Would the percent composition for a drop of water be different from that of a swimming pool full of pure water?

C. Determine the empirical formulas of the compounds given their percent composition by mass.

1) 82.66% carbon, 17.34% hydrogen
2) 69.94% iron, 30.06% oxygen
3) 78.14% boron, 21.86% hydrogen
4) 24.42% calcium, 17.07% nitrogen, 58.50% oxygen
5) 25.85% potassium, 42.41% sulphur, 31.74% oxygen
6) 40.00% carbon, 6.71% hydrogen, 53.29% oxygen

D. Determine the molecular formulas for the compounds from C given these molar masses (the molar mass from D1 goes with C1 and so on).

1) 58.124 g/mol
2) 159.69 g/mol
3) 27.67 g/mol
4) 164.092 g/mol
5) 302.460 g/mol
6) 180.162 g/mol

E. Determine the unknown elements in each compound given the percent compositions and molar masses. Write the correct form of the chemical formula.

1) AB : 67.10% A and 32.90% B, molar mass = 97.475 g/mol
2) A_2B_2: 71.51% A and 28.49% B, molar mass = 560.99 g/mol
3) A_3B: 85.82% A and 14.18% B, molar mass = 48.962 g/mol
4) A_3BC: 89.09% A, 10.06% B and 0.84% C, molar mass = 119.378 g/mol
5) A_3B_4C: 42.07% A, 39.04% B and 18.89% C, molar mass = 163.940 g/mol

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SOLUTIONS

A: (1) 46.7% silicon, 53.3% oxygen (2) 74.9% carbon, 25.1% hydrogen (3) 60.0% potassium, 18.4% carbon, 21.5% nitrogen (4) 100% oxygen (5) 41.1% nitrogen, 11.8% hydrogen, 47.1% sulphur (6) 49.5% carbon, 5.2% hydrogen, 28.9% nitrogen, 16.5% oxygen

B: (1) No, because the composition of water is the same as that for steam. (2) Yes, because the proportion of hydrogen to oxygen is different in H_2O_2. (3) No, because percent composition describes the ratio of elements in a substance, not overall quantity. Water is water.

C: (1) C_2H_5 (2) Fe_2O_3 (3) BH_3 (4) CaN_2O_6 (5) KS_2O_3 (6) CH_2O

D: (1) C_4H_{10} (2) Fe_2O_3 (3) B_2H_6 (4) CaN_2O_6 (or $Ca(NO_3)_2$) (5) $K_2S_4O_6$ (6) $C_6H_{12}O_6$

E: (1) A = zinc, B = sulphur; ZnS (2) A = mercury, B = bromine; Hg_2Br_2
(3) A = nitrogen, B = lithium; LiN_3
(4) A = chlorine, B = carbon, C = hydrogen; $CC\ell_3H$
(5) A = sodium, B = oxygen, C = phosphorus; Na_3PO_4