Moles

Skills to Develop

- Define a mole
- Distinguish theoretical yield from actual yield

Moles are a convenient unit used in chemistry to convert between amounts of a substance in grams and numbers of atoms or molecules. This is useful because we usually measure how much of a molecule is used or produced in a reaction by massing it, but as a chemical equation shows, the reaction will happen between atoms or molecules. For example, suppose we combine 1.0 g of calcium oxide (CaO) with 1.0 g of water (H_2O). The product we get is $Ca(OH)_2$. Here's the equation:

$$CaO(s) + H_2O(l) \rightarrow Ca(OH)_2(s \text{ or } aq) \tag{1}$$

This is balanced. Thus every molecule of water reacts with one CaO formula unit (it's not called a molecule because it's an ionic solid, and each Ca^{2+} ion is surrounded with oxide ions that it interacts with equally). How much calcium hydroxide is produced by this reaction? Once all of one reactant has been used, whatever is left of the other will stop reacting, because of the law of definite proportions: we won't change the ratio of O:H:Ca in the product. So will we get solid calcium hydroxide with calcium oxide left over, or will we have water left over, and thus get $Ca(OH)_2(aq)$? To answer this question, we can convert both masses (1 g of each) to the number of molecules or formula weights, but this would be inconvenient because the number would be very very big!

Instead, we use **moles**. A mole (abbreviation: mol) is like a pair, which means 2 of something. You can have a pair of people, a pair of apples, whatever. A mole is 6.022 x 10^{23} of something. This is a convenient quantity because it converts amu (atomic mass units) to grams. The atomic weight of carbon is (on average) 12.011 amu/atom. It is also 12.011g/mol. In other words, 1g = 6.02 x 10^{23} amu. Usually, a mol of a substance is a useful, practical amount, somewhere between a few grams and a few kg. The number of things in a mole, 6.022 x 10^{23}, is called Avogadro's number, and abbreviated as N_A. It is named after Avogadro, the scientist who proposed that a liter of any gas at the same temperature and pressure has the same number of molecules in it. To summarize:

1 mole of [thing] = N_A things = 6.022 x 10^{23} things

So the way to answer the question above is to convert both quantities to moles. The maximum amount of product that can be formed is the smaller number of moles. The formula weight is just the sum of the atomic weights.

$$(1.0 \;\; g\, \cancel{CaO}) \left(\frac{1 \;\; mol\, \cancel{CaO}}{56.08 \;\; g\, \cancel{CaO}} \right) \left(\frac{10^3 \; mmol\, CaO}{1 \;\; mol\, \cancel{CaO}} \right) = 17.8 \; mmol\, CaO \tag{2}$$

$$(1.0 \;\; g\, \cancel{H_2O}) \left(\frac{1 \;\; mol\, \cancel{H_2O}}{18.01 \;\; g\, \cancel{H_2O}} \right) \left(\frac{10^3 \; mmol\, H_2O}{1 \;\; mol\, \cancel{H_2O}} \right) = 55.5 \; mmol\, H_2O \tag{3}$$

After we make 17.8 mmol (milimoles) of $Ca(OH)_2$, we will use up all the CaO, so the reaction won't continue. The maximum amount of $Ca(OH)_2$ possible to make is 17.8 mmol. If we wanted to know the **theoretical yield** (maximum mass of product) of $Ca(OH)_2$, we could do it in a one-step calculation like this:

$$(1.0 \;\; g\, \cancel{CaO}) \left(\frac{1 \;\; mol\, \cancel{CaO}}{56.08 \;\; g\, \cancel{CaO}} \right) \left(\frac{1 \;\; mol\, \cancel{Ca(OH)_2}}{1 \;\; mol\, \cancel{CaO}} \right) \left(\frac{74.09 \; g\, Ca(OH)_2}{1 \;\; mol\, \cancel{Ca(OH)_2}} \right) = 1.3 \; g\, Ca(OH)_2 \tag{4}$$

Here, we knew that the **limiting reactant** (or limiting reagent), which is the reactant that will run out first, is CaO because the masses are the same, the coefficients in the equation are the same, and the formula weight of CaO is bigger than the molecular weight of water. So we start with the limiting reactant mass, convert it to moles (using 1 mol = 56.08 g), then "convert" between moles of CaO and moles of $Ca(OH)_2$ using the coefficients from the balanced equation (1 mol of CaO produces 1 mol of $Ca(OH)_2$), then we convert to g of $Ca(OH)_2$ (using 1 mol = 74.09 g). This is just an example of using dimensional analysis to convert units. We check to make sure we have always multiplied by 1 (because 1 mol CaO = 56g CaO, so (1 mol CaO/56 g CaO)=1), and that the units cancel out to leave the correct final units (g $Ca(OH)_2$), and we can be pretty sure that we got it right.

Here's a slightly more complicated example. This time, we add 2.0 g of water to 2.5 g of Li_2O. This will produce LiOH as the major product. What is the most LiOH (in g) that could be produced, also called the theoretical yield?

To answer, first we need to write and balance the chemical equation. It's going to look pretty similar to the previous one, because this is a similar reaction.

$$Li_2O(s) + H_2O(l) \rightarrow 2LiOH(s \ or \ aq) \tag{5}$$

Which is the limiting reactant? The formula weights are 18.01 g and 29.88 g. Water is still in **excess**, which means it will be left over. Here's the unit conversion:

$$(2.5 \ \ g \ \cancel{Li_2O}) \left(\frac{1 \ \ mol \ \cancel{Li_2O}}{29.88 \ \ g \ \cancel{Li_2O}} \right) \left(\frac{2 \ \ mol \ \cancel{LiOH}}{1 \ \ mol \ \cancel{Li_2O}} \right) \left(\frac{23.95 \ g \ LiOH}{1 \ \ mol \ \cancel{LiOH}} \right) = 4.0 \ g \ LiOH \tag{6}$$

Note

This time we used 1 mol Li_2O producing 2 mol LiOH, using the coefficients from the balanced equation.

Outside Links

- Khan Academy: The Mole and Avogadro's Number (10 min)
- Khan Academy: Molecular and Empirical Formulas (15 min)
- CrashCourse Chemistry: Stoichiometry (13 min)

Contributors and Attributions

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