How can you use moles to calculate the number of atoms in a sample of material?

You can use the mole concept to calculate how many particles make up the mass of a sample of material. In order to perform the calculation, you need to know the molar mass. **Molar mass** is the mass of one mole of the material. If the representative particle of a material is an atom, then the molar mass (in grams per mole) is numerically equal to atomic mass (in atomic mass units). As you see in Figure 1, each box on the periodic table gives the atomic mass of the element.

The atomic mass for a single atom of aluminum is 26.982 atomic mass units. The following calculation shows how to use an element’s atomic mass in the conversion of mass to number of atoms. Suppose you needed to find the number of atoms in 7.85 g of aluminum. As shown below, first you would convert the mass to moles, and then you would convert the moles to atoms.

\[
7.85 \text{ g Al} \times \frac{1 \text{ mol Al}}{26.982 \text{ g Al}} \times \frac{6.02 \times 10^{23} \text{ Al atoms}}{1 \text{ mol Al}} = 1.75 \times 10^{23} \text{ Al atoms}
\]

You can also perform the inverse calculation and determine the mass of a given number of atoms of a material. Suppose you needed to find the mass of a certain number of atoms of magnesium. As shown below, first convert the number of atoms to moles. Then use the atomic mass of magnesium (atomic mass = 24.305) to find the mass of the moles.

\[
4.38 \times 10^{23} \text{ Mg atoms} \times \frac{1 \text{ mol Mg}}{6.02 \times 10^{23} \text{ Mg atoms}} \times \frac{24.305 \text{ g Mg}}{1 \text{ mol Mg}} = 17.7 \text{ g Mg}
\]

In both of these calculations, the key is to convert the quantity you know into moles. From moles, it is often easier to convert into other units.
How can you use moles to calculate the number of molecules or formula units in a sample of material?

The representative particle for a molecular compound is a molecule, and the representative particle for an ionic compound is a formula unit. In order to calculate the number of molecules or formula units that make up a given mass of a compound, you also have to know the compound’s formula. The formula identifies the number of atoms or ions in each representative unit. The following are examples:

- Each formula unit of iron bromide (FeBr₉) consists of one iron ion (Fe²⁺) and two bromide ions (Br⁻).
- Each molecule of ammonia (NH₃) consists of one atom of nitrogen (N) and three atoms of hydrogen (H).

To calculate molar mass, recognize that a mole of Mg₃N₂ will contain three moles of magnesium and two moles of nitrogen. You can add these masses to determine the molar mass of a single mole of Mg₃N₂.

\[
3 \text{ mol Mg} \times \frac{24.305 \text{ g Mg}}{1 \text{ mol Mg}} = 72.915 \text{ g}
\]

\[
2 \text{ mol N} \times \frac{14.007 \text{ g N}}{1 \text{ mol N}} = 28.014 \text{ g}
\]

\[
\text{molar mass Mg₃N₂} = 100.929 \text{ g/mol}
\]

After you know the molar mass of the compound, you can calculate the number of molecules or ions from the mass of the compound, as shown in the example below for 16.2 g of the ionic compound magnesium nitride:

\[
16.2 \text{ g Mg₃N₂} \times \frac{1 \text{ mol Mg₃N₂}}{100.929 \text{ g Mg₃N₂}} \times \frac{6.02 \times 10^{23} \text{ mol Mg₃N₂ formula units}}{1 \text{ mol Mg₃N₂}} = 9.66 \times 10^{22} \text{ Mg₃N₂ formula units}
\]

First you calculate the number of moles by dividing the mass of the sample by the molar mass of the compound. You then calculate the number of formula units by multiplying by Avogadro’s number.

If you wanted to, you could also perform the inverse calculations to determine the mass of a sample if you know the number of molecules or ions. To solve for this, you would divide by Avogadro’s number to solve for moles and then multiply the result by the compound’s molar mass to solve for mass.
How can you use moles to calculate the number of ions in a sample of material?

You can also use a compound’s formula to calculate the number of particles other than representative particles. In this case, you have to multiply by the subscript of the atom or ion in which you are interested. The following example shows how to calculate the number of ions in 16.2 g of magnesium nitride.

\[
16.2 \text{ g Mg}_3\text{N}_2 \times \frac{1}{100.929 \text{ g Mg}_3\text{N}_2} \times \frac{3 \text{ mol Mg}}{1 \text{ mol Mg}_3\text{N}_2} \times \frac{6.02 \times 10^{23} \text{ Mg}^- \text{ ions}}{1 \text{ mol Mg}} = 2.90 \times 10^{23} \text{ Mg}^- \text{ ions}
\]

End-of-Course Assessment Review

1. Define The molar mass of Al\(_2\)Cl\(_6\) is the mass of one mole of the compound. It is also which of the following?
   A the mass of 1 mole of Al and 1 mole of Cl
   B the mass of 2 moles of Al and 6 moles of Cl
   C the mass of 1/2 mole of Al and 1/2 mole of Cl
   D the mass of 1/4 mole of Al and 3/4 mole of Cl

2. Calculate How many atoms make up 3.29 g of silicon (Si)?
   A \(2.14 \times 10^{22}\)
   B \(7.05 \times 10^{22}\)
   C \(6.02 \times 10^{23}\)
   D \(1.98 \times 10^{24}\)

3. Calculate How many molecules make up 12.8 g of N\(_2\)O\(_4\)?
   A \(8.37 \times 10^{22}\)
   B \(5.02 \times 10^{23}\)
   C \(7.71 \times 10^{24}\)
   D \(7.09 \times 10^{26}\)

4. Construct Write a step-by-step procedure for converting the mass of an ionic compound to the number of formula units that make up the compound.

5. Evaluate A student calculates the number of chloride ions (Cl\(^-\)) in 7.0 g of aluminum chloride (AlCl\(_3\)). He incorrectly states that the answer is \(3.16 \times 10^{22}\) Cl\(^-\) ions. What mistake did the student most likely make? What is the correct answer?
How can you determine mass relationships between reactants and products?

The calculation of quantities in chemical reactions is a subject of chemistry called **stoichiometry**. Calculations using balanced equations are called stoichiometric calculations. When preparing chemicals for a reaction, chemists often measure the mass of each reactant. A balanced chemical equation, however, describes the relationships among moles of each substance. To describe mass relationships for the reaction, one must first calculate the molar mass of each reactant and product, and then use the molar masses to convert between moles and grams.

**Sample Problem 1**

Suppose, for example, 8.75 g of propane (C₃H₈) react with oxygen gas (O₂) to produce carbon dioxide (CO₂) and water (H₂O). How many grams of water are produced?

First, write and balance a chemical equation for the reaction:

\[ \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \]

Calculate the molar masses of propane and water.

- **propane**: \(3(12.011 \text{ g/mol}) + 8(1.008 \text{ g/mol}) = 44.097 \text{ g/mol}\)
- **water**: \(2(1.008 \text{ g/mol}) + 1(15.999 \text{ g/mol}) = 18.015 \text{ g/mol}\)

List what you know:

- mass of propane = 8.75 g
- \(4 \text{ mol H}_2\text{O} \quad 1 \text{ mol C}_3\text{H}_8\)

Start with a given quantity and convert from mass to moles.

\[
8.75 \text{ g C}_3\text{H}_8 \times \frac{1 \text{ mol C}_3\text{H}_8}{44.097 \text{ g C}_3\text{H}_8}
\]

Then convert from moles of reactant to moles of product:

\[
8.75 \text{ g C}_3\text{H}_8 \times \frac{1 \text{ mol C}_3\text{H}_8}{44.097 \text{ g C}_3\text{H}_8} \times \frac{4 \text{ mol H}_2\text{O}}{1 \text{ mol C}_3\text{H}_8}
\]

Finish by converting moles to grams using the molar mass of water.

\[
8.75 \text{ g C}_3\text{H}_8 \times \frac{1 \text{ mol C}_3\text{H}_8}{44.097 \text{ g C}_3\text{H}_8} \times \frac{4 \text{ mol H}_2\text{O}}{1 \text{ mol C}_3\text{H}_8} \times \frac{18.015 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}} = 14.3 \text{ g H}_2\text{O}
\]

Vocabulary

- stoichiometry
- limiting reagent
- excess reagent
- theoretical yield
- actual yield
- percent yield
How can you determine the limiting reagent in a reaction?

The **limiting reagent** in a chemical reaction is the reactant that determines the amount of each product that will form. When all of the limiting reagent has been used, the reaction stops. Any other reactants that remain are **excess reagents**. In Figure 1, the hydrogen gas (H\(_2\)) is the limiting reagent because it is used up in the reaction. The oxygen gas (O\(_2\)) is the excess reagent because some of it does not get used in the reaction.

**Figure 1**
Gas as the Limiting Reagent in the Synthesis of Water

<table>
<thead>
<tr>
<th>Before reaction</th>
<th>After reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 H(_2) and 7 O(_2)</td>
<td>10 H(_2)O and 2 O(_2)</td>
</tr>
</tbody>
</table>

**Study Tip**
Remember that the limiting reagent is the reactant that produces the only possible amount of the product given the reactants available.

If you know the mass or number of moles of each reactant, you can use the chemical equation to determine the limiting reagent. First, choose one of the reactants. Then use coefficients of the chemical equation and atomic masses to determine how much of each of the other reactants would be needed to completely use up the available mass of the first reactant. The reactant with the least available mass compared to how much is needed is the limiting reagent.

**Sample Problem 2**
For example what is the limiting reagent when 385 g of sodium (Na) reacts with 125 g of chlorine gas (Cl\(_2\))? Write the balanced equation for the reaction:

\[
2Na + Cl\_2 \rightarrow 2NaCl
\]

List what you know and what you need to solve for.

- mass of sodium = 385 g
- mass of chlorine gas = 125 g Cl\(_2\)

\[
\frac{1 \text{ mol } Cl\_2}{2 \text{ mol } Na}
\]

Start with a given quantity and convert from mass to moles.

\[
385 \text{ g Na} \times \frac{1 \text{ mol Na}}{22.990 \text{ g Na}}
\]

Then convert from moles of reactant to moles of product:

\[
385 \text{ g Na} \times \frac{1 \text{ mol Na}}{22.990 \text{ g Na}} \times \frac{1 \text{ mol Cl}\_2}{2 \text{ mol Na}}
\]

Determine the amount of Cl\(_2\) that would react with 385 g of Na.

\[
385 \text{ g Na} \times \frac{1 \text{ mol Na}}{22.990 \text{ g Na}} \times \frac{1 \text{ mol Cl}\_2}{2 \text{ mol Na}} \times \frac{70.906 \text{ g Cl}\_2}{1 \text{ mol Cl}\_2} = 594 \text{ g Cl}\_2
\]

Since only 125 g of chlorine gas (instead of 594 g) is available, it must be the limiting reagent. Sodium is the excess reagent.
How can you calculate percent yield?
The amount of a product that you calculate is actually a theoretical yield. Frequently, however, reactions do not run to completion and some reactants remain unused. The amount of a product that actually forms is the actual yield. The ratio of actual yield to theoretical yield, multiplied by 100 percent, is the percent yield.

\[
\text{percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%
\]

Suppose, for example, that you calculate a theoretical yield of 58.2 g, but the actual yield is 51.9 g. The percent yield is:

\[
\text{percent yield} = \frac{51.9 \text{ g}}{58.2 \text{ g}} \times 100\% = 89.2\%
\]

End-of-Course Assessment Review

1. Calculate Which of the following reactions had the greatest percent yield?
   A theoretical yield 52.3 g; actual yield 50.7 g
   B theoretical yield 17.1 g; actual yield 15.7 g
   C theoretical yield 38.8 g; actual yield 36.2 g
   D theoretical yield 24.6 g; actual yield 22.5 g

2. Predict What is the mass of Br₂ that will form if 5.35 g of KBr reacts with excess Cl₂? The chemical equation is Cl₂ + 2KBr → 2KCl + Br₂?
   A 1.80 g
   B 2.68 g
   C 3.59 g
   D 7.18 g

3. Evaluate The equation 3Mg × N₂ → Mg₃N₂ describes the synthesis of magnesium nitride (Mg₃N₂). In a specific example, 2.6 moles of magnesium (Mg) and 4.5 moles of nitrogen gas (N₂) are combined to form magnesium nitride (Mg₃N₂). A student concludes that Mg is the limiting reagent. Do you agree? Defend your answer.