



How to calculate theoretical yield chemistry

Each product has a theoretical yield, meaning the amount of product you would expect to get if the reaction is perfectly efficient.[7] Continuing the example above, you are analyzing the reaction $6 O 2 + C 6 H 12 O 6 \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6CO_{2} + 6H_{2} O \} \}$. The equation is balanced. Question What should I do if there is more than one reactant? As a more complicated example, oxygen and glucose can react to form carbon dioxide and water: $6 O 2 + C 6 H 12 O 6 \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6CO_{2} + 6H_{2} O \} \}$. The equation is balanced. Question What should I do if there is more than one reactant? As a more complicated example, oxygen and glucose can react to form carbon dioxide and water: $6 O 2 + C 6 H 12 O 6 \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6CO_{2} + 6H_{2} O \} \}$. hydrogen (H) atoms, and 18 oxygen (O) atoms. 25g C 6 H 12 O 6 {\displaystyle C_{6}H_{12}O_{6}} / (180 g/mol) = about 0.139 moles of glucose. The molar mass of one atom of oxygen is about 16 g/mol. Thus, the other reactant, glucose in this case, is the limiting reactant. Therefore, beginning with 0.139 moles of glucose should result in 0.834 moles of water. The ratio of carbon dioxide to glucose is 6:1. Return to the balanced equation. For an actual experiment, you will know the mass in grams of each reactant that you are using. The other reactant, glucose (C 6 H 12 O 6 {\displaystyle C {6}H {12}O {6}}) has a molar mass of (6 atoms C x 12 g C/mol) + (12 atoms H x 1 g H/mol) + (6 atoms O x 16 g O/mol) = 180 g/mol. If you try to compare the mass of each, you will not reach the correct results.[8] In the example above, glucose is the limiting reactant. The one that gets used up first is called the limiting reactant. Co-authors: 15 Updated: February 10, 2025 Views: 1,189,309 Categories: Chemistry Calculations Print Send fan mail to authors Thanks to all authors for creating a page that has been read 1,189,309 times. Bess Ruff is a Geography PhD student at Florida State University. 5 Convert the result to grams. A mole is a tool used in chemistry to count molecules, based on their mass. A chemical equation is like a recipe. 1 Start with a balanced chemical equation. It shows the reactants (on the left side) reacting to form products (on the right side). Multiplying by the product, this results in 0.834 moles H2O x 18 g/mol H2O = ~15 grams. This equation tells you that you expect 6 molecules of the desired product, carbon dioxide (CO2 {\displaystyle CO {2}}), compared to 1 molecule of glucose (C 6 H 12 O 6 {\displaystyle C {6}H {12}O {6}}). 2 Write down the number of moles of your limiting reactant. In some cases, you may be concerned only with one product or the other. In other words, this reaction can produce 6 molecules of carbon dioxide from one molecule of glucose. When you know the number of moles that you expect, you will multiply by the molar mass of the product to find the theoretical yield in grams.[11] In this example, the molar mass of CO2 is about 44 g/mol. In this example, the second product is water, H 2 O {\displaystyle H_{2}O}. To find the ratio between the two, divide the number of moles of one reactant by the number of moles of mole the other.[4] In this example, you are starting with 1.25 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen and 0.139 moles of glucose. The ideal ratio for this reaction is 6 oxygen atoms x 16 g/mol per atom = 32 g/mol of O 2 {\displaystyle O_{2}}. This change has corrected the oxygen, which now has two atoms on both sides. The theoretical yield of carbon dioxide is (0.139 moles glucose) x (6 moles carbon dioxide is (0.139 moles glucose) = 0.834 moles carbon dioxide. Advertisement 1 Review the reaction to find the desired product. The right side of a chemical equation shows the products created by the reaction. The molar mass is 2 + 16 = 18 g/mol. She has conducted survey work for marine spatial planning projects in the Caribbean and provided research support as a graduate fellow for the Sustainable Fisheries Group. In the next step, you need to compare it to the ideal molar ratio from your chemical equation to find the limiting reactant and continue as described in the article. Using the periodic table or some other reference, look up the molar mass of each atom in each compound. 2 Calculate the molar mass of each reactant. 3 Compare the ratio of molecules in product and reactant. One molecule of glucose plus six molecules of oxygen = six molecules of water plus six molecules of carbon dioxide. Therefore, you have more oxygen than required. The two atoms of hydrogen on both the left and right. The coefficients in front of each molecule tell you the ratio of the molecules that you need for the reaction to occur. In most chemical reactants will be used up before the others. 40 g O 2 {\displaystyle O {2}} / (32 g/mol) = 1.25 moles of oxygen. Add them together to find the molar mass of each compound of reactant. Compare the two ratios you calculated to identify the limiting reactant:[6] In this example, you are beginning with 9 times as much oxygen as glucose, when measured by number of moles. She received her MA in Environmental Science and Management from the balanced equation for the reaction. Multiply the number of moles of water by the molar mass of water. Question What should I do if the reactants have the same number of moles? Find out which of the reactants is the "limiting" reactant and use that to calculate the theoretical yield. A properly balanced equation will show the same number of atoms going into the equation as reactants as you have coming out in the form of products.[1] For example, consider the simple equation H 2 + O 2 {\displaystyle H {2}+O {2}} \rightarrow H 2 O {\displaystyle H {2}+O {2} \rightarrow H 2 O {\displaystyle H {2}+O {2} and water: $6 O 2 + C 6 H 12 O 6 \{(displaystyle 6O_{2}+C_{6}H_{12}O_{6}\} \rightarrow 6 C O 2 + 6 H 2 O \{(displaystyle 6CO_{2}+6H_{2}O)\}$ For this example, one molecule of oxygen ($O 2 \{(displaystyle O_{2})\}$) contains two oxygen atoms. You must always compare moles of reactant to moles of product. The theoretical yield of water for this experiment is 15 grams. If you wish to find the theoretical yield of both products, just repeat the process. Thus, the ratio of oxygen to glucose molecules is 1.25 / 0.139 = 9.0. This ratio means that you have 9 times as many molecules of oxygen as you have of glucose. (Carbon's molar mass is ~12 g/mol and oxygen's is ~16 g/mol, so the total is 12 + 16 + 16 = 44.) Multiply 0.834 moles CO2 x 44 g/mol CO2 = ~36.7 grams. The theoretical yield of the experiment is 36.7 grams of CO2. This can be done using Part 1 of this article. If you use exactly the ratio given by the formula, then both reactants should be used equally.[5] For this reaction, the reactants are given as 6 O 2 + C 6 H 12 O 6 {\displaystyle $6O_{2}+C_{6}H_{12}O_{6}$. This limiting reactant determines how long the chemical reaction can take place and the theoretical yield you can expect. This will adjust the equation to 2 H 2 + O 2 {\displaystyle 2H_{2}} - 2 H 2 O {\displaystyle 2H_{2}}. Yes. This is the reverse of your earlier step of calculating the number of moles or reactant. The ratio of carbon dioxide to glucose is 6/1 = 6. 4 Determine the molar ratio of the reactants. "This explained it better than my actual chemical equation. But there are two atoms of oxygen going in as a reactant and only one atom in the product on the right. The coefficients of each product, if the reaction is balanced, tells you the amount to expect, in molecular ratios. Advertisement 3 Convert the amount of 6:1. The answer is the theoretical yield, in moles, of the desired product.[10] In this example, the 25g of glucose equate to 0.139 moles of glucose. This change now has 4 atoms of hydrogen on both sides, and two atoms of oxygen. 6 Repeat the calculation for the other product if desired. Divide this value by that compound's molar mass to convert the amount to moles.[3] For example, suppose you begin with 40 grams of oxygen and 25 grams of glucose. Divide the number of molecules of your desired product by the number of molecules of your limiting reactant.[9] The balanced equation for this example is $6 O 2 + C 6 H 12 O 6 \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \} \rightarrow 6 C O 2 + 6 H 2 O \{ \text{displaystyle } 6O_{2} + C_{6} H_{12} O_{6} \} \}$ on the left with four atoms of hydrogen on the right. That's not a problem! It only means that the molar ratio of your reactants is 1. The molar mass calculations found that the initial 25g of glucose are equal to 0.139 moles of glucose. You can begin with either product to calculate theoretical yield. To balance, double the product, to get H 2 + O 2 $dsplaystyle H_{2}+O_{2} \rightarrow 2 H 2 O$ See more answers Ask a Question Advertisement This article was co-authored by Bess Ruff, MA. The coefficients indicate that you need 6 oxygen molecules for every 1 glucose molecule. 4 Multiply the ratio by the limiting reactant's quantity in moles. If so, that is the one you would start with. Advertisement Add New Question Doesn't one molecule of glucose produce six molecules of water, not one? In many experiments, you may only be concerned with the yield of one product. The formula tells you that your ideal ratio is 6 times as much oxygen as glucose. You expect to create six times as many moles of carbon dioxide as you have of glucose to begin with. According to the balanced equation, you expect 6 molecules of water to come from 1 molecule of glucose. Check the balance.

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