

About Percent Yield in the Organic Laboratory

Definitions: **Theoretical Yield:** The maximum amount of product if ALL of the limiting reagent reacted exactly as described by the balanced equation, with no losses due to side reactions or spillage.

Percent Yield: The amount of purified product obtained, divided by the theoretical yield. A Percent Yield over 100% is physically impossible -- as far as we know, you cannot create matter...if you do, please let your instructor know right away so we can nominate you for the next Nobel Prize in chemistry!!

Crude Percent Yield: Percent yield of the crude product before purification. This crude material may contain product, starting material, byproducts from side reactions, moisture, and a variety of other impurities. Therefore this number may be over 100%. The amounts of such impurities are more characteristic of the technical details of the operation or the technical skill level of the operator than the nature of the reaction itself, so this number is rarely published in the chemical literature.

Purified Percent Yield: *See Percent Yield.* These are the same. If the chemical literature refers to percent yield, without stating "purified", it is assumed that the product was pure.

Percent Recovery: This describes the efficiency of purification operations such as recrystallization, where the identity of the material is the same before and after the operation. To calculate, divide the amount obtained by the amount which entered the operation, times 100 to express in percent. The molecular weight doesn't change, so units of grams may be used.

How to calculate: First calculate the theoretical yield, then use it in the other calculations.

(LR = limiting reagent, P = product, MW = molecular weight in g/mol)

$$\text{Theoretical yield (g)} = (\text{amount of LR}) \cdot (\text{MW of P}) \cdot \left(\frac{\text{moles of P}}{\text{moles of LR}} \right)$$

amount actually used in reaction, in moles (points to amount of LR)

stoichiometric ratio from balanced equation (for many organic reactions this is 1:1) (points to moles of P / moles of LR)

this is the amount of purified product obtained (points to amount of P (g) in the percent yield equation)

$$\text{Percent yield} = \text{purified percent yield} = \frac{\text{amount of P (g)}}{\text{theoretical yield (g)}} \cdot 100$$
$$\text{Crude percent yield} = \frac{\text{amount of crude P before purification (g)}}{\text{theoretical yield (g)}} \cdot 100$$

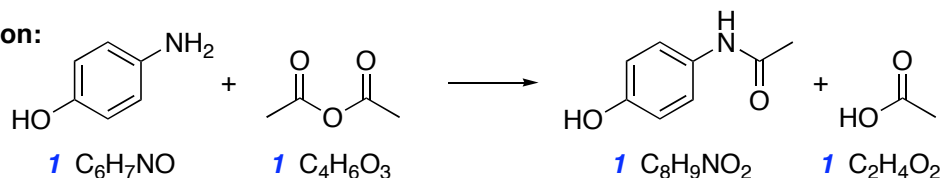
Complicated balanced equations are uncommon in organic chemistry. Many organic reactions have a stoichiometry of 1:1 in the balanced equation. In this case the calculation can be further simplified; the theoretical yield calculation may be skipped. But the amounts must still be converted to moles!

$$\text{Percent yield (if stoichiometry is 1:1)} = \frac{\text{amount of P (mol)}}{\text{amount of LR (mol)}} \cdot 100$$

Yield Calculations: Example

Arthur Rytis prepared acetaminophen in the Organic Lab. Starting with 2.14 g of *p*-aminophenol, and 1.9 mL acetic anhydride, Arthur obtained 3.22 g crude product. After setting aside a sample of the crude product for TLC analysis, Arthur purified 2.88 g of the crude product by recrystallization. *Note that not all of the crude product was recrystallized; the fraction used was 2.88/3.22 = 0.894.* The recrystallized product weighed 2.43 g.

Balance the equation:



The stoichiometry here is 1:1: 1 mol of limiting reagent gives 1 mol product

Find the limiting reagent: Since this balanced reaction has a 1:1 stoichiometry, the limiting reagent is simply the lower amount (in moles) of these two compounds

for *p*-aminophenol,

$$\frac{2.14 \text{ g}}{109 \text{ g/mol}} = 0.0196 \text{ mol}$$

for acetic anhydride,

$$\frac{(1.9 \text{ mL}) \cdot (1.08 \text{ g/mL})}{102 \text{ g/mol}} = 0.0201 \text{ mol}$$

(note that the density is used to convert the volume of acetic anhydride to mass)

so, *p*-aminophenol is the limiting reagent (LR)

Calculate theoretical yield: $\text{Theoretical yield (g)} = (\text{moles of LR}) \cdot \left(\frac{\text{g P}}{\text{mole P}} \right) \cdot \left(\frac{\text{moles of P}}{\text{moles of LR}} \right)$

$= (0.0196 \text{ mol}) \cdot (151 \text{ g/mol}) \cdot \left(\frac{1}{1} \right) = 2.96 \text{ g}$

(An arrow points from the text "MW of P" to the 151 g/mol term in the calculation.)

Calculate Percent Yield: Since not all of the crude product was recrystallized, we need to account for that in the calculation of percent yield. In other words, the percent yield should reflect what you would have gotten if you purified the whole batch. Calculate in the usual way, then divide by the fraction used for recrystallization.

$$\text{Percent yield} = \frac{2.43 \text{ g}}{2.96 \text{ g}} \cdot 100 / 0.894 = 92\%$$

(An arrow points from the text "dividing by the fraction used in the recrystallization" to the 0.894 term in the calculation.)

An alternative way to calculate this, when not all the crude is purified, is to consider the formation of crude product and purification to be individual steps, then the overall yield is obtained by multiplying the yields of the two steps. This method also accounts for the fact that only a fraction was used for recrystallization.

$$\text{Crude percent yield} = \frac{3.22 \text{ g}}{2.96 \text{ g}} \cdot 100 = 109\%$$

$$\text{Percent recovery from recrystallization} = \frac{2.43 \text{ g}}{2.88 \text{ g}} \cdot 100 = 84\%$$

$$\text{Percent yield} = 1.09 \cdot 0.84 \cdot 100 = 92\% \quad \text{(this is the same answer obtained above)}$$