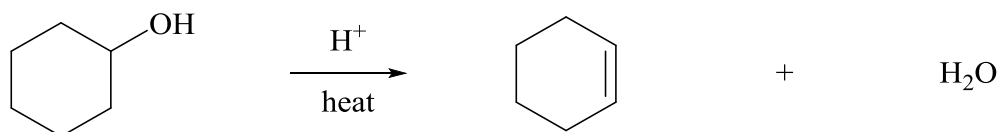


## Percent Yield Calculations

Dehydration of Cyclohexanol to Cyclohexene.

**Theoretical yield.** First write out the balanced equation. This is a very simple case. One reactant produces one product (water is also a product but we are only interested in the cyclohexene here) in a 1:1 ratio. Note that the phosphoric acid is a catalyst and is not involved in the yield calculation.



One molecule of cyclohexanol should produce one molecule of cyclohexene. One mole (mol) of cyclohexanol should produce one mole of cyclohexene.

If 2.05 g of cyclohexanol is used (use the actual amount used in your experiment) convert this to moles by dividing by the molecular weight of cyclohexanol (MW = 100.2 g/mol).

$$2.05 \text{ g cyclohexanol} / 100.2 \text{ g/mol} = 0.0205 \text{ mol (or 20.5 mmol)}$$

Because 1 mol of cyclohexanol should produce 1 mol of cyclohexene, 0.0205 mol of cyclohexanol should produce 0.0205 mol of cyclohexene. Convert this number of moles of cyclohexene to grams of cyclohexene by multiplying by the MW of cyclohexene (82.1 g/mol).

$$0.0205 \text{ mol} \times 82.1 \text{ g/mol} = 1.68 \text{ g cyclohexene}$$

In other words, 2.05 g of cyclohexanol should produce 1.68 g of cyclohexene. This is the best-case yield also known as the **theoretical yield**.

**Percent Yield.** The theoretical yield is what would be obtained in an ideal world, if every molecule of cyclohexanol were converted to a molecule of cyclohexene. The percent yield is the percentage of the theoretical yield that you actually obtain after isolating product at the end of the procedure.

Let's say that after the final fractional distillation of the cyclohexene, 1.22 g was collected. The percent yield then would be

$$\text{percent yield} = (\text{actual} / \text{theoretical}) \times 100 = (1.22 \text{ g} / 1.68 \text{ g}) \times 100 = 73 \%$$

This assumes that the 1.22 g that was obtained was 100% pure. Let's say that when the gas chromatographic analysis was done the sample was found to be 89% cyclohexene and 11% toluene. This means that the 1.22 g of liquid isolated in the distillation was not pure cyclohexene. The actual amount of cyclohexene collected then was  $1.22 \text{ g} \times 0.89 = 1.09 \text{ g}$  (small print: an assumption is being made: that the gc detector response is the same for cyclohexene and toluene. We will accept this assumption for our purposes. In fact it is a good assumption in this case). The percent yield then would be:

$$(1.09 \text{ g actual} / 1.68 \text{ g theoretical}) \times 100 = 65\%.$$