

5.4: Yield And Atom Economy in Chemical Reactions

A fundamental concept basic to green chemistry that can be illustrated by chemical reactions is the distinction between yield and atom economy. In Chapter 2 *yield* was defined as a percentage of the degree to which a chemical reaction or synthesis goes to completion and *atom economy* was defined as the fraction of reactants that go into final products. Those two ideas are illustrated here for the preparation of HCl gas which, dissolved in water, produces hydrochloric acid. There are several ways in which HCl can be prepared. One of these commonly used in the laboratory is the reaction of concentrated sulfuric acid, H₂SO₄, with common table salt, NaCl, accompanied by heating to drive off the volatile HCl vapor:



This reaction can be performed so that all of the NaCl and H₂SO₄ react, which gives a 100% yield. But it produces Na₂SO₄ byproduct, so the atom economy is less than 100%. The percent atom economy is calculated very simply by the relationship

$$\text{Percent atom economy} = \frac{\text{Mass of desired product}}{\text{Total mass of product}} \times 100 \quad (5.4.2)$$

(We could just as well divide by the total mass of reactants since in a chemical reaction it is equal to the total mass of products.) In this case, the mass of the desired product is that of 2 HCl and the total mass of product is that of 2HCl + Na₂SO₄. Given the atomic masses H 1.0, Cl 35.5, Na 23.0, and O 16.0 gives the following:

$$\text{Mass of desired product} = 2 \times (1.0 + 35.5) = 73.0 \quad (5.4.3)$$

$$\text{Total mass product} = 2 \times (1.0 + 35.5) + (2 \times 23.0 + 32.0 + 4 \times 16.0) = 215 \quad (5.4.4)$$

$$\text{Percent atom economy} = \frac{73.0}{215} \times 100 = 34.0\% \quad (5.4.5)$$

This result shows that even with 100% yield, the reaction is only 34.0% atom economical and if it were used as a means to prepare HCl large quantities of Na₂SO₄, a material with only limited value, would be produced. In contrast, the direct reaction of hydrogen gas with chlorine gas to give HCl gas,



can be carried out with 100% atom economy if all of the H₂ reacts with Cl₂. There is no waste byproduct.

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