Chapter 10
Chemical Calculations and Chemical Equations

An Introduction to Chemistry
by Mark Bishop

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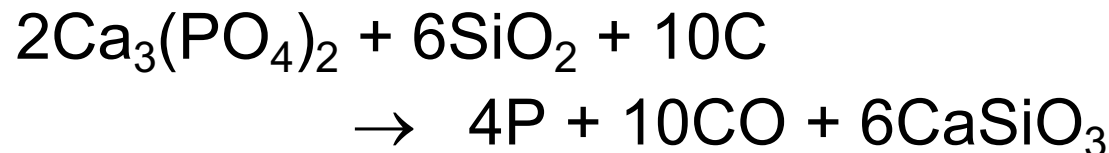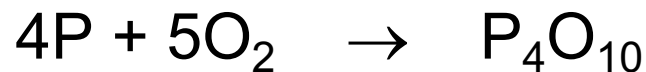
Making Phosphoric Acid

- Furnace Process for making H_3PO_4 to be used to make fertilizers, detergents, and pharmaceuticals.
    - React phosphate rock with sand and coke at 2000 ºC.

    $$2Ca_3(PO_4)_2 + 6SiO_2 + 10C$$
    $$\rightarrow \quad 4P + 10CO + 6CaSiO_3$$

    - React phosphorus with oxygen to get tetraphosphorus decoxide.

    $$4P + 5O_2 \quad \rightarrow \quad P_4O_{10}$$

    - React tetraphosphorus decoxide with water to make phosphoric acid.

    $$P_4O_{10} + 6H_2O \quad \rightarrow \quad 4H_3PO_4$$

Sample Calculation

- What is the minimum mass of water that must be added to 2.50×10^4 kg P_4O_{10} to form phosphoric acid in the following reaction?

$$P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$$

Goal: To develop conversion factors that will convert between a measurable property (mass) and number of particles

Measurable Property 1   Mass 1

↓   ↓

Number of Particles 1   Moles 1

↓   ↓

Number of Particles 2   Moles 2
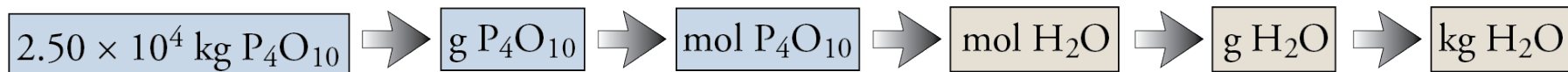
↓   ↓

Measurable Property 2   Mass 2

Two Very Similar Calculations

- Conversion between amount of compound and amount of element in that compound (from Section 6.7 of the atoms-first version of the text and Section 9.4 of the chemistry-first version).

$$1.09 \times 10^4 \text{ kg P} \Rightarrow \text{g P} \Rightarrow \text{mol P} \Rightarrow \text{mol P}_4\text{O}_{10} \Rightarrow \text{g P}_4\text{O}_{10} \Rightarrow \text{kg P}_4\text{O}_{10}$$
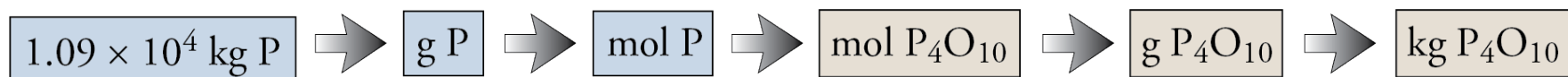
$$? \text{ kg P}_4\text{O}_{10} = 1.09 \times 10^4 \text{ kg P} \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol P}}{30.9738 \text{ g P}} \right) \left(\frac{1 \text{ mol P}_4\text{O}_{10}}{4 \text{ mol P}} \right) \left(\frac{283.889 \text{ g P}_4\text{O}_{10}}{1 \text{ mol P}_4\text{O}_{10}} \right) \left(\frac{1 \text{ kg}}{10^3 \text{ g}} \right)$$

$$= 2.50 \times 10^4 \text{ kg P}_4\text{O}_{10}$$

- Conversion between units of one substance and units of another substance, both involved in a chemical reaction.

$$2.50 \times 10^4 \text{ kg P}_4\text{O}_{10} \Rightarrow \text{g P}_4\text{O}_{10} \Rightarrow \text{mol P}_4\text{O}_{10} \Rightarrow \text{mol H}_2\text{O} \Rightarrow \text{g H}_2\text{O} \Rightarrow \text{kg H}_2\text{O}$$

$$? \text{ kg H}_2\text{O} = 2.50 \times 10^4 \text{ kg P}_4\text{O}_{10} \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol P}_4\text{O}_{10}}{283.889 \text{ g P}_4\text{O}_{10}} \right) \left(\frac{6 \text{ mol H}_2\text{O}}{1 \text{ mol P}_4\text{O}_{10}} \right) \left(\frac{18.0153 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}} \right) \left(\frac{1 \text{ kg}}{10^3 \text{ g}} \right)$$

$$= 9.52 \times 10^3 \text{ kg H}_2\text{O}$$

Molar Ratio from Coefficients in Balanced Equations

$$P_4O_{10} \quad + \quad 6H_2O \quad \rightarrow \quad 4H_3PO_4$$
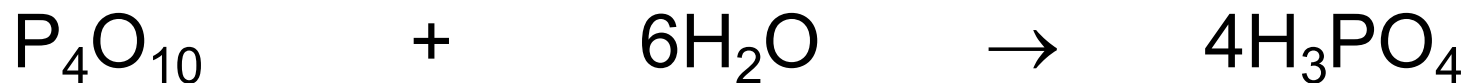
1 molecule P_4O_{10}	6 molecules H_2O	4 molecules H_3PO_4
1 dozen P_4O_{10} molecules	6 dozen H_2O molecules	4 dozen H_3PO_4 molecules
6.022×10^{23} molecules P_4O_{10}	$6(6.022\times10^{23})$ molecules H_2O	$4(6.022\times10^{23})$ molecules H_3PO_4
1 mole P_4O_{10}	6 moles H_2O	4 moles H_3PO_4

Sample Calculations (2)

- What is the minimum mass of water that must be added to 2.50×10^4 kg P_4O_{10} to form phosphoric acid in the following reaction?

$$P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$$

- The coefficients in the balanced equation provide us with a conversion factor that converts from units of P_4O_{10} to units of H_2O.

$$\left(\frac{1 \text{ mol } P_4O_{10}}{6 \text{ mol } H_2O}\right) \qquad \left(\frac{1 \text{ mol } P_4O_{10}}{4 \text{ mol } H_3PO_4}\right) \qquad \left(\frac{6 \text{ mol } H_2O}{4 \text{ mol } H_3PO_4}\right)$$

Sample Calculation

- What is the minimum mass of water that must be added to 2.50×10^4 kg P_4O_{10} to form phosphoric acid in the following reaction?

$$P_4O_{10} + 6H_2O \;\rightarrow\; 4H_3PO_4$$

$$? \text{ kg } H_2O = 2.50 \times 10^4 \text{ kg } P_4O_{10} \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol } P_4O_{10}}{283.889 \text{ g } P_4O_{10}} \right) \left(\frac{6 \text{ mol } H_2O}{1 \text{ mol } P_4O_{10}} \right) \left(\frac{18.0153 \text{ g } H_2O}{1 \text{ mol } H_2O} \right) \left(\frac{1 \text{ kg}}{10^3 \text{ g}} \right)$$

$$= 9.52 \times 10^3 \text{ kg } H_2O$$

Equation Stoichiometry

- **Tip-off -** The calculation calls for you to convert from amount of one substance to amount of another, both of which are involved in a chemical reaction.

- **General Steps**

1. If you are not given it, write and balance the chemical equation for the reaction.
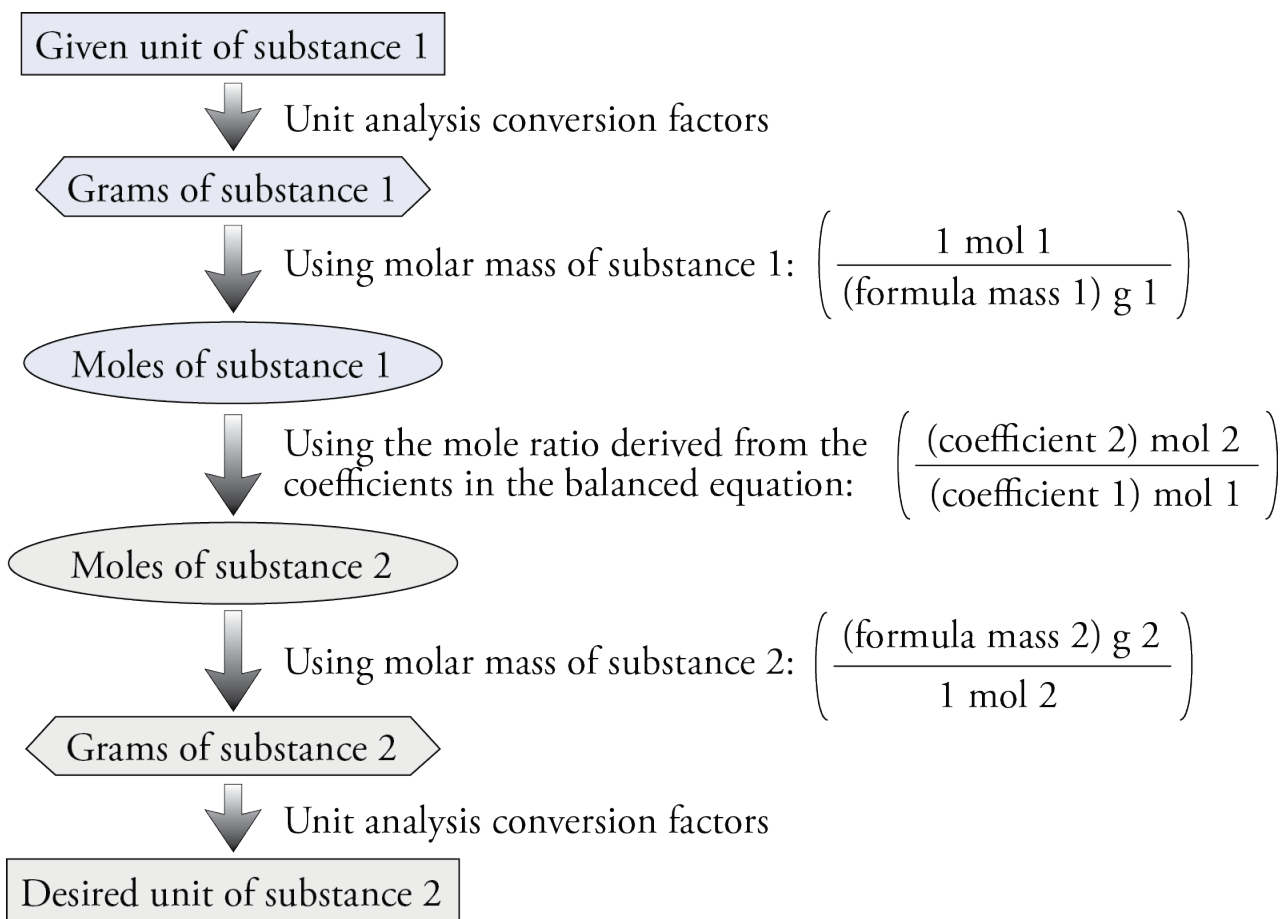
Equation Stoichiometry

2. Start your unit analysis in the usual way.

3. If you are not given grams of substance 1, convert from the unit that you are given to grams. This may take one or more conversion factors.

4. Convert from grams of substance 1 to moles of substance 1.

Equation Stoichiometry

5. Convert from moles of substance 1 to moles of substance 2 using the coefficients from the balanced equation to create the molar ratio used as a conversion factor.

6. Convert from moles of substance 2 to grams of substance 2, using its molar mass.

7. If necessary, convert from grams of 2 to the desired unit for 2. This may take one or more conversion factors.
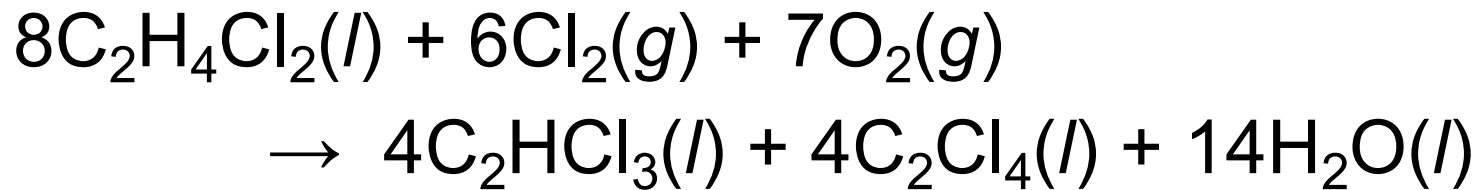
Equation Stoichiometry Steps

Given unit of substance 1

⬇ Unit analysis conversion factors

Grams of substance 1

⬇ Using molar mass of substance 1: $\left(\dfrac{1\ \text{mol}\ 1}{(\text{formula mass}\ 1)\ \text{g}\ 1} \right)$

Moles of substance 1

⬇ Using the mole ratio derived from the coefficients in the balanced equation: $\left(\dfrac{(\text{coefficient}\ 2)\ \text{mol}\ 2}{(\text{coefficient}\ 1)\ \text{mol}\ 1} \right)$

Moles of substance 2

⬇ Using molar mass of substance 2: $\left(\dfrac{(\text{formula mass}\ 2)\ \text{g}\ 2}{1\ \text{mol}\ 2} \right)$

Grams of substance 2

⬇ Unit analysis conversion factors

Desired unit of substance 2

Equation Stoichiometry Steps

Molar mass of substance 2

$$? \text{ (unit) 2} = \text{(given) (unit) 1} \left(\frac{\text{--- g}}{\text{--- (unit)}}\right)\left(\frac{\text{1 mol 1}}{\text{--- g 1}}\right)\left(\frac{\text{(coefficient 2) mol 2}}{\text{(coefficient 1) mol 1}}\right)\left(\frac{\text{--- g 2}}{\text{1 mol 2}}\right)\left(\frac{\text{--- (unit)}}{\text{--- g}}\right)$$
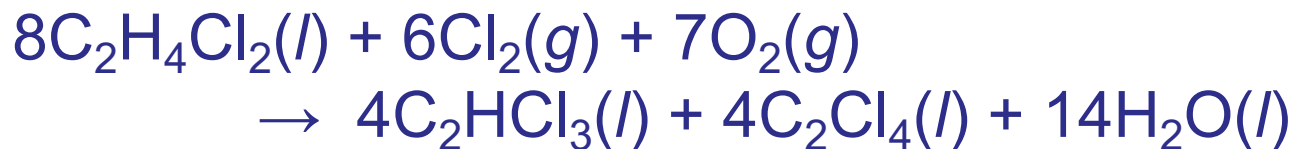
One or more conversion factors convert the given unit to grams.

Molar mass of substance 1

One or more conversion factors convert grams to the given unit.

Sample Calculation

- Tetrachloroethene, C_2Cl_4, often called perchloroethylene (perc), is a colorless liquid used in dry cleaning. It can be formed in several steps from the reaction of d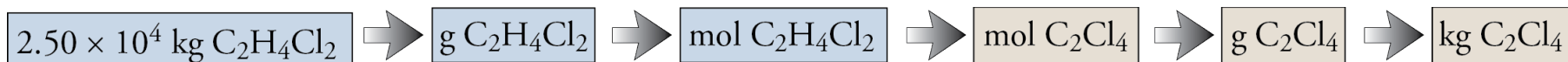ichloroethane, chlorine gas, and oxygen gas. What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:
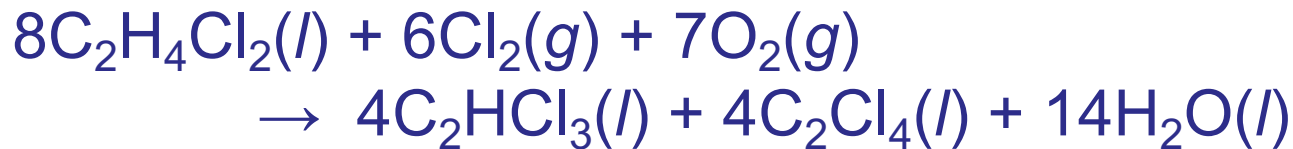
$$8C_2H_4Cl_2(l) + 6Cl_2(g) + 7O_2(g)$$
$$\rightarrow \ 4C_2HCl_3(l) + 4C_2Cl_4(l) + 14H_2O(l)$$

What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:

$$8C_2H_4Cl_2(l) + 6Cl_2(g) + 7O_2(g)$$
$$\rightarrow 4C_2HCl_3(l) + 4C_2Cl_4(l) + 14H_2O(l)$$

- Usual unit analysis steps

$$? \text{ kg } C_2Cl_4 = 23.75 \cancel{\text{ kg}} \text{ } C_2H_4Cl_2 \left(\frac{}{\cancel{\text{kg}}} \right)$$

- Tip-off: The calculation calls for you to convert from amount of one substance to amount of another, both of which are involved in a chemical reaction.

| 2.50×10^4 kg $C_2H_4Cl_2$ | ⇨ | g $C_2H_4Cl_2$ | ⇨ | mol $C_2H_4Cl_2$ | ⇨ | mol C_2Cl_4 | ⇨ | g C_2Cl_4 | ⇨ | kg C_2Cl_4 |

What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:

$$8C_2H_4Cl_2(l) + 6Cl_2(g) + 7O_2(g)$$
$$\rightarrow 4C_2HCl_3(l) + 4C_2Cl_4(l) + 14H_2O(l)$$

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right)$$

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{}{\text{g } C_2H_4Cl_2} \right)$$
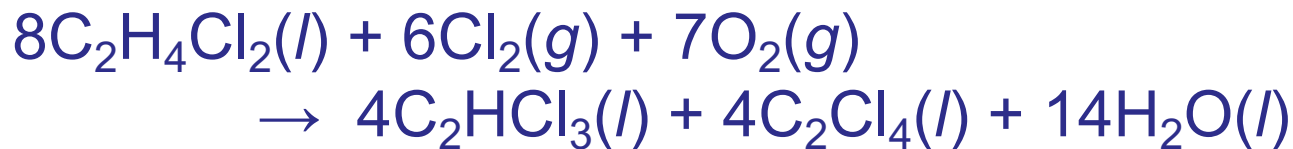
$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right)$$

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\frac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\frac{}{\text{mol } C_2H_4Cl_2} \right)$$

What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:

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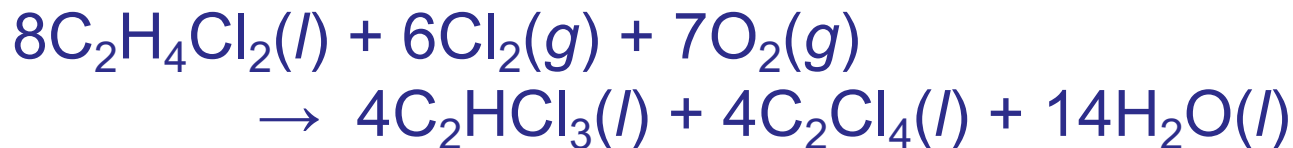
$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\dfrac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\dfrac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\dfrac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right)$
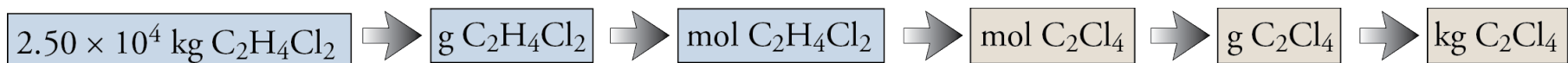
$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\dfrac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\dfrac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\dfrac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right) \left(\dfrac{}{\text{mol } C_2Cl_4} \right)$

$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\dfrac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\dfrac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\dfrac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right) \left(\dfrac{165.833 \text{ g } C_2Cl_4}{1 \text{ mol } C_2Cl_4} \right)$

$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\dfrac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\dfrac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\dfrac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right) \left(\dfrac{165.833 \text{ g } C_2Cl_4}{1 \text{ mol } C_2Cl_4} \right) \left(\dfrac{}{\text{g}} \right)$

$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\dfrac{10^3 \text{ g}}{1 \text{ kg}} \right) \left(\dfrac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right) \left(\dfrac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right) \left(\dfrac{165.833 \text{ g } C_2Cl_4}{1 \text{ mol } C_2Cl_4} \right) \left(\dfrac{1 \text{ kg}}{10^3 \text{ g}} \right)$

What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:

$$8C_2H_4Cl_2(l) + 6Cl_2(g) + 7O_2(g)$$
$$\rightarrow 4C_2HCl_3(l) + 4C_2Cl_4(l) + 14H_2O(l)$$

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{10^3 \text{ g}}{1 \text{ kg}} \right)\left(\frac{1 \text{ mol } C_2H_4Cl_2}{98.959 \text{ g } C_2H_4Cl_2} \right)\left(\frac{4 \text{ mol } C_2Cl_4}{8 \text{ mol } C_2H_4Cl_2} \right)\left(\frac{165.833 \text{ g } C_2Cl_4}{1 \text{ mol } C_2Cl_4} \right)\left(\frac{1 \text{ kg}}{10^3 \text{ g}} \right)$$

$$= \textbf{19.90 kg } C_2Cl_4$$

2.50×10^4 kg $C_2H_4Cl_2$ ⇒ g $C_2H_4Cl_2$ ⇒ mol $C_2H_4Cl_2$ ⇒ mol C_2Cl_4 ⇒ g C_2Cl_4 ⇒ kg C_2Cl_4

Equation Stoichiometry Shortcut for Mass-Mass Problems

Given mass of substance 1

Using $\left(\dfrac{\text{(coefficient 2) (formula mass 2) (any mass unit) substance 2}}{\text{(coefficient 1) (formula mass 1) (same mass unit) substance 1}} \right)$

Same mass unit of substance 2

$? \text{ (unit) 2} = \text{(given) (unit) 1} \left(\dfrac{\text{(coefficient 2) (formula mass 2) (any mass unit) substance 2}}{\text{(coefficient 1) (formula mass 1) (same mass unit) substance 1}} \right)$

What is the maximum mass of perchloroethylene, C_2Cl_4, that can be formed from 23.75 kilograms of dichloroethane, $C_2H_4Cl_2$? The equation for the net reaction is:

$$8C_2H_4Cl_2(l) + 6Cl_2(g) + 7O_2(g)$$
$$\rightarrow 4C_2HCl_3(l) + 4C_2Cl_4(l) + 14H_2O(l)$$
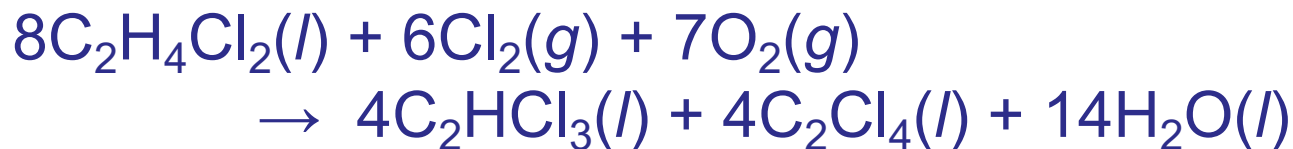
- Usual unit analysis steps

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{}{\text{kg}} \right)$$

- Tip-off: The calculation calls for you to convert from mass of one substance to mass of another, both of which are involved in a chemical reaction.

- We can use the shortcut.

$$? \text{ kg } C_2Cl_4 = 23.75 \text{ kg } C_2H_4Cl_2 \left(\frac{4 \times 165.833 \text{ kg } C_2Cl_4}{8 \times 98.959 \text{ kg } C_2H_4Cl_2} \right)$$

$$= \textbf{19.90 kg } \mathbf{C_2Cl_4}$$

Questions to Ask When Designing a Process for Making a Substance

- How much of each reactant should be added to the reaction vessel?

- What level of purity is desired for the final product? If the product is mixed with other substances (such as excess reactants), how will this purity be achieved?

Limiting Component

$+$ $\rightarrow$
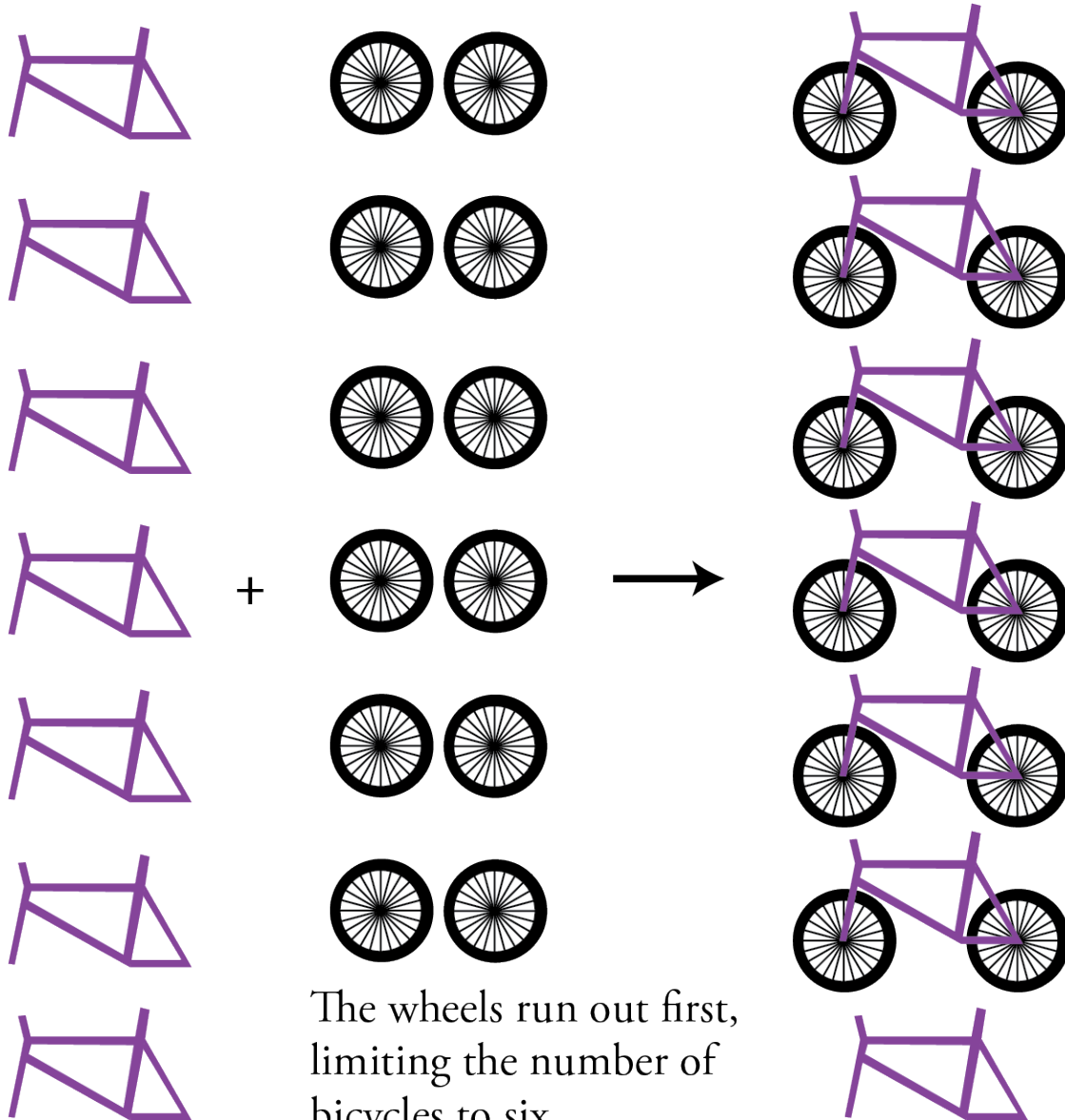
The wheels run out first, limiting the number of bicycles to six.

The frames are in excess.

Why substance limiting? (1)

- To ensure that one reactant is converted to products most completely.
  - Expense

$$P_4(s) + 5O_2(g) \rightarrow P_4O_{10}(s) + \text{excess } O_2(g)$$

  - Importance

$$SiO_2(s) + 2C(s)$$
$$\rightarrow Si(l) + 2CO(g) + \text{excess } C(s)$$

Why substance limiting? (2)

- Concern for excess reactant that remains
  - danger

$P_4(s) + 5O_2(g) \rightarrow P_4O_{10}(s)$ + excess $O_2(g)$

  - ease of separation

$SiO_2(s) + 2C(s)$

$\rightarrow Si(l) + 2CO(g)$ + excess $C(s)$

Limiting Component
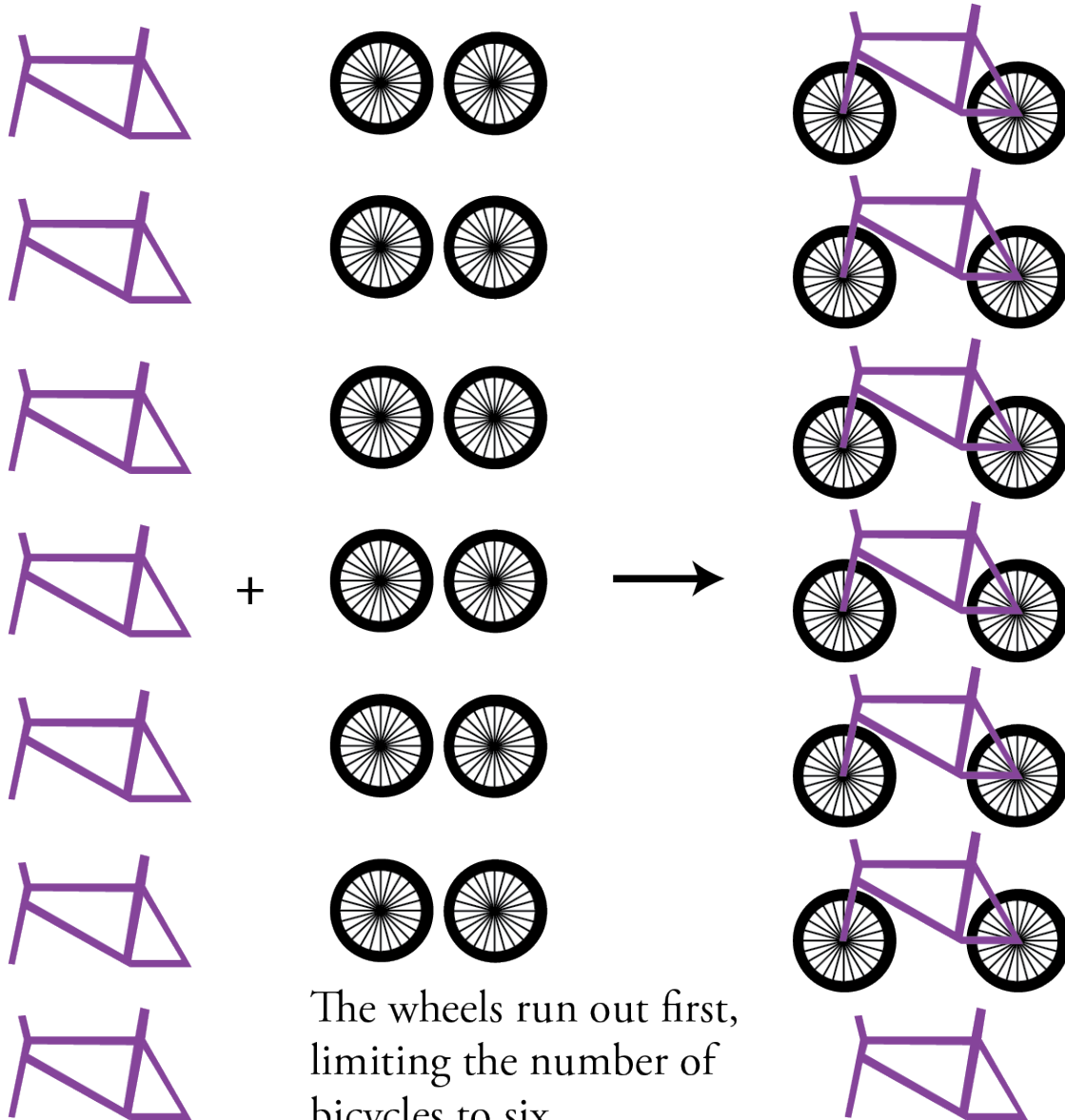
The wheels run out first, limiting the number of bicycles to six.

The frames are in excess.

Limiting Component (2)

$$\left(\frac{1 \text{ bicycle}}{1 \text{ frame}}\right) \quad \text{and} \quad \left(\frac{1 \text{ bicycle}}{2 \text{ wheels}}\right)$$

$$? \text{ bicycles} = 7 \text{ frames} \left(\frac{1 \text{ bicycle}}{1 \text{ frame}}\right) = 7 \text{ bicycles}$$

$$? \text{ bicycles} = 12 \text{ wheels} \left(\frac{1 \text{ bicycle}}{2 \text{ wheels}}\right) = 6 \text{ bicycles}$$

Limiting Reactant

- The reactant that runs out first in a chemical reaction limits the amount of product that can form. This reactant is called the *limiting reactant*.

Limiting Reactant Problems

- **Tip-off -** You are given amounts of two or more reactants in a chemical reaction, and you are asked to calculate the maximum amount of a product that can form from the combination of the reactants.

- **General Steps**

1. Do separate calculations of the maximum amount of product that can form from each reactant.

2. The lowest of the values calculated in the step above is your answer. It is the maximum amount of product that can be formed from the given amounts of reactants.

Example

- The uranium(IV) oxide, UO_2, used as fuel in nuclear power plants has a higher percentage of the fissionable isotope uranium-235 than is present in the UO_2 found in nature. To make fuel grade UO_2, chemists first convert uranium oxides to uranium hexafluoride, UF_6, whose concentration of uranium-235 can be increased by a process described in my online lecture for Section 16.3 of the atoms-first version of my text and Section 18.3 of the chemistry-first version. The enriched UF_6 is then converted back to UO_2 in a series of reactions, beginning with

  $$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF$$
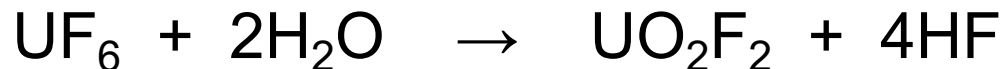
  a. How many megagrams of UO_2F_2 can be formed from the reaction of 24.543 Mg UF_6 with 8.0 Mg of water?

 b. Why do you think the reactant in excess was chosen to be in excess?

Example
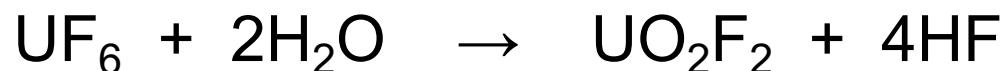
$$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF$$

How many megagrams of UO_2F_2 can be formed from the reaction of 24.543 Mg UF_6 with 8.0 Mg of water?

- Limiting reactant tip-off – We are given amounts of two reactants and asked to calculate an amount of product.

- Steps
  - Calculate amount of UO_2F_2 from 24.543 Mg UF_6.
  - Calculate amount of UO_2F_2 from 8.0 Mg of H_2O.
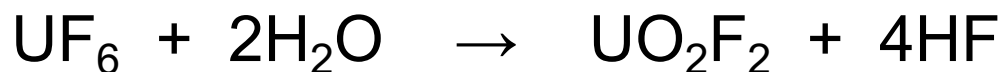 - Smaller value is answer.

Example
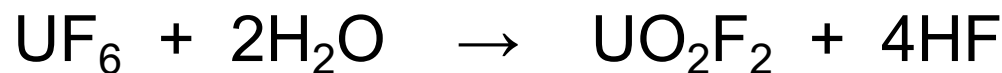
$$UF_6 \; + \; 2H_2O \;\; \rightarrow \;\; UO_2F_2 \; + \; 4HF$$

How many megagrams of UO_2F_2 can be formed from the reaction of 24.543 Mg UF_6 with 8.0 Mg of water?

? Mg UO_2F_2 = 24.543 Mg UF_6

? Mg UO_2F_2 = 24.543 Mg UF_6 $\left(\dfrac{1 \times \quad\quad\quad\quad}{1 \times \quad\quad\quad\quad} \right)$

? Mg UO_2F_2 = 24.543 Mg UF_6 $\left(\dfrac{1 \times 308.0245}{1 \times 352.019} \right)$
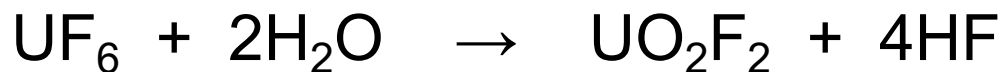
Example

$$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF$$

How many megagrams of UO_2F_2 can be formed from the reaction of 24.543 Mg UF_6 with 8.0 Mg of water?

$$? \text{ Mg } UO_2F_2 = 24.543 \text{ Mg } UF_6 \left(\frac{1 \times 308.0245 \text{ Mg}}{1 \times 352.019 \text{ Mg}} \right)$$

$$? \text{ Mg } UO_2F_2 = 24.543 \text{ } \cancel{\text{Mg } UF_6} \left(\frac{1 \times 308.0245 \text{ Mg } UO_2F_2}{1 \times 352.019 \text{ } \cancel{\text{Mg } UF_6}} \right)$$

$$? \text{ Mg } UO_2F_2 = 24.543 \text{ } \cancel{\text{Mg } UF_6} \left(\frac{1 \times 308.0245 \text{ Mg } UO_2F_2}{1 \times 352.019 \text{ } \cancel{\text{Mg } UF_6}} \right)$$

$$= 21.476 \text{ Mg } UO_2F_2$$

Example

$$UF_6 + 2H_2O \rightarrow UO_2F_2 + 4HF$$

How many megagrams of UO_2F_2 can be formed from the reaction of 24.543 Mg UF_6 with 8.0 Mg of water?

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$$= 21.476 \text{ Mg } UO_2F_2$$

$$? \text{ Mg } UO_2F_2 = 8.0 \text{ Mg } H_2O \left(\frac{1 \times 308.0245 \text{ Mg } UO_2F_2}{2 \times 18.0153 \text{ Mg } H_2O} \right)$$

$$= 68 \text{ Mg } UO_2F_2$$

Example

b. Why do you think the reactant in excess was chosen to be in excess?
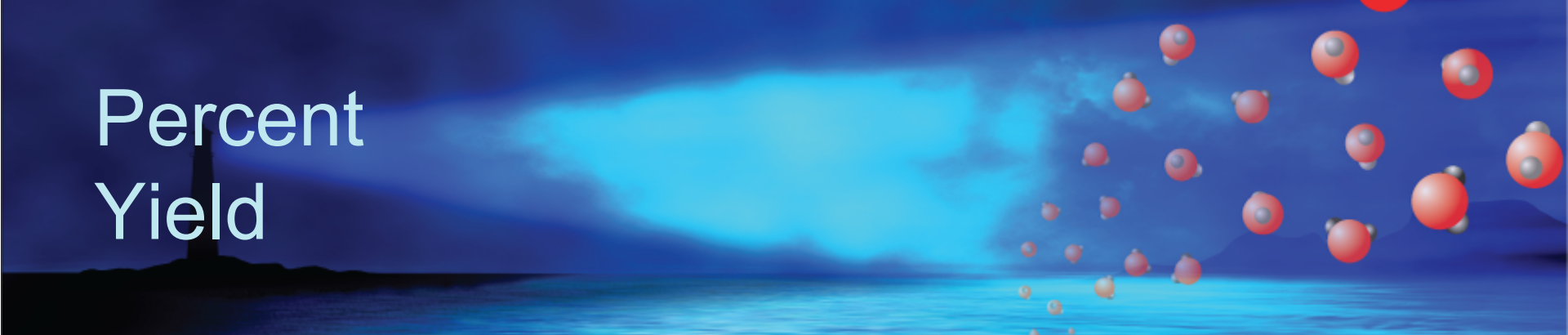
- – Water is much less expensive than the rare uranium compound.

- – It is important to carry as much uranium through the process as possible.

- – It is better to have the nontoxic water in the final mixture than the radioactive UF_6.

- – Water is also easy to separate from the solid product mixture.

Why not 100% Yield?

- Reversible reactions

- Side reactions

- Slow reactions

- Loss during separation/purification

Percent Yield

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$

- **Actual yield** is measured. It is given in the problem.

- **Theoretical yield** is the maximum yield that you calculate.

Example Calculation for Percent Yield

- Sodium chromate, Na_2CrO_4, is made by roasting chromite, $FeCr_2O_4$, with sodium carbonate, Na_2CO_3. (Roasting means heating in the presence of air or oxygen.) A simplified version of the net reaction is
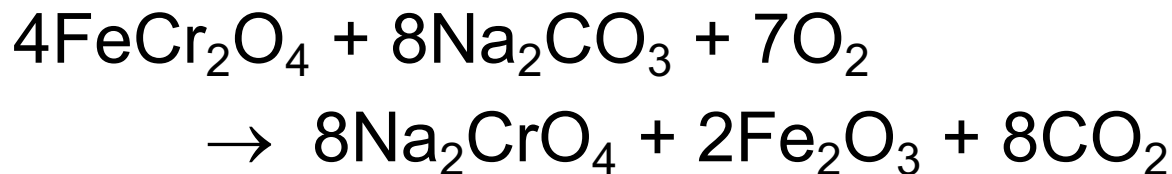
$$4FeCr_2O_4 + 8Na_2CO_3 + 7O_2$$
$$\rightarrow 8Na_2CrO_4 + 2Fe_2O_3 + 8CO_2$$

- What is the percent yield if 1.2 kg of Na_2CrO_4 is produced from ore that contains 1.0 kg of $FeCr_2O_4$?

Example Calculation for Percent Yield
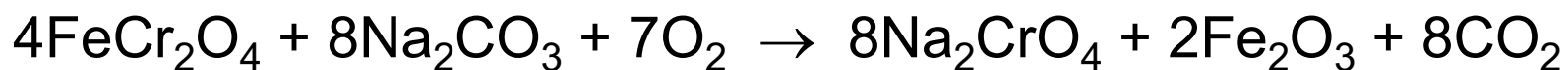
$4FeCr_2O_4 + 8Na_2CO_3 + 7O_2 \rightarrow 8Na_2CrO_4 + 2Fe_2O_3 + 8CO_2$

What is the percent yield if 1.2 kg of Na_2CrO_4 is produced from ore that contains 1.0 kg of $FeCr_2O_4$?

$$\text{Percent Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%$$

- Na_2CrO_4 is a product, so 1.2 kg Na_2CrO_4 is the *actual yield*.
- $FeCr_2O_4$ is a reactant, so 1.0 kg $FeCr_2O_4$ is used to calculate the maximum amount of Na_2CrO_4 that could be formed (the *theoretical yield*).

Example Calculation for Percent Yield
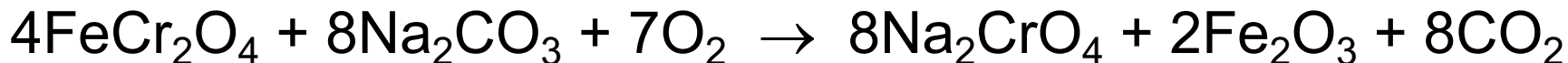
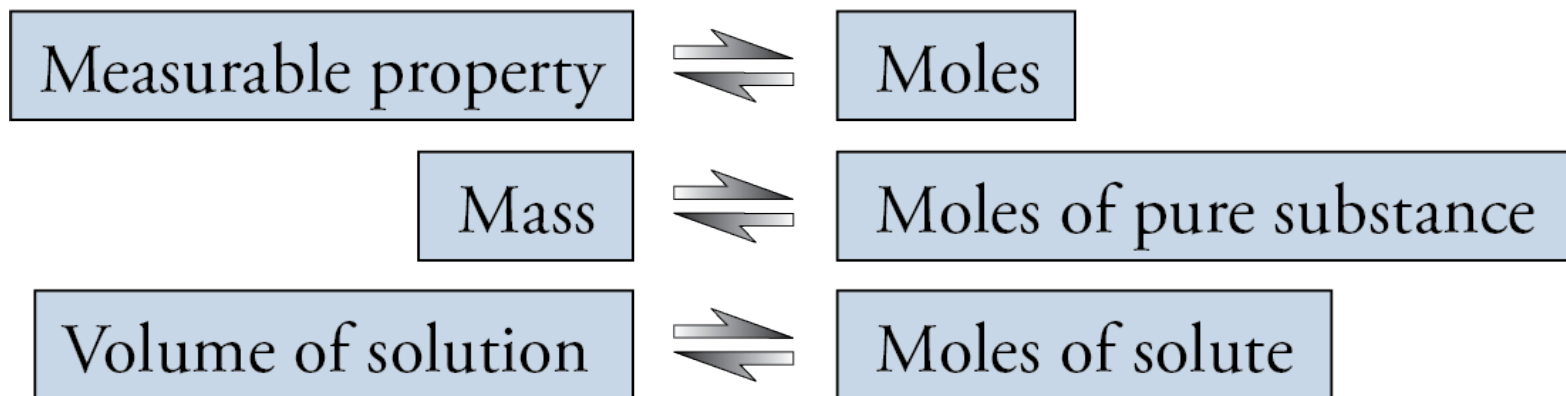$4FeCr_2O_4 + 8Na_2CO_3 + 7O_2 \rightarrow 8Na_2CrO_4 + 2Fe_2O_3 + 8CO_2$

- What is the percent yield if 1.2 kg of Na_2CrO_4 is produced from ore that contains 1.0 kg of $FeCr_2O_4$?

$$? \text{ kg } Na_2CrO_4 = 1.0 \text{ kg } FeCr_2O_4 \left(\frac{10^3 \text{ g}}{1 \text{ kg}}\right)\left(\frac{1 \text{ mol } FeCr_2O_4}{223.835 \text{ g } FeCr_2O_4}\right)\left(\frac{8 \text{ mol } Na_2CrO_4}{4 \text{ mol } FeCr_2O_4}\right)\left(\frac{161.9733 \text{ g } Na_2CrO_4}{1 \text{ mol } Na_2CrO_4}\right)\left(\frac{1 \text{ kg}}{10^3 \text{ g}}\right)$$

$$= 1.4 \text{ kg } Na_2CrO_4$$

$$\text{Percent yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

$$= \frac{1.2 \text{ kg } Na_2CrO_4}{1.4 \text{ kg } Na_2CrO_4} \times 100\% = \mathbf{86\% \ yield}$$

Conversions to Moles

Measurable property	⇌	Moles
Mass	⇌	Moles of pure substance
Volume of solution	⇌	Moles of solute

Molarity

$$\text{Molarity} = \frac{\text{moles of solute}}{\text{liter of solution}}$$

- Converts between moles of solute and volume of solution

$$0.500 \text{ M Na}_3\text{PO}_4 \text{ means } \frac{0.500 \text{ mol Na}_3\text{PO}_4}{1 \text{ L Na}_3\text{PO}_4 \text{ solution}} \text{ or } \frac{0.500 \text{ mol Na}_3\text{PO}_4}{10^3 \text{ mL Na}_3\text{PO}_4 \text{ solution}}$$

Calculating Molarity

- A silver perchlorate solution was made by dissolving 29.993 g of pure $AgClO_4$ in water and then diluting the mixture with additional water to achieve a total volume of 50.00 mL. What is the solution's molarity?

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Calculating Molarity

- A silver perchlorate solution was made by dissolving 29.993 g of pure $AgClO_4$ in water and then diluting the mixture with additional water to achieve a total volume of 50.00 mL. What is the solution's molarity?

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$$? \text{ M } AgClO_4 = \frac{? \text{ mol } AgClO_4}{1 \text{ L } AgClO_4 \text{ soln}} = \frac{29.993 \text{ g } \cancel{AgClO_4}}{50.00 \text{ } \cancel{mL} \text{ } AgClO_4 \text{ soln}} \left(\frac{1 \text{ mol } AgClO_4}{207.3185 \text{ g } \cancel{AgClO_4}} \right) \left(\frac{10^3 \text{ } \cancel{mL}}{1 \text{ L}} \right)$$

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$$= \frac{2.893 \text{ mol } AgClO_4}{1 \text{ L } AgClO_4 \text{ soln}} = \textbf{2.893 M } AgClO_4$$
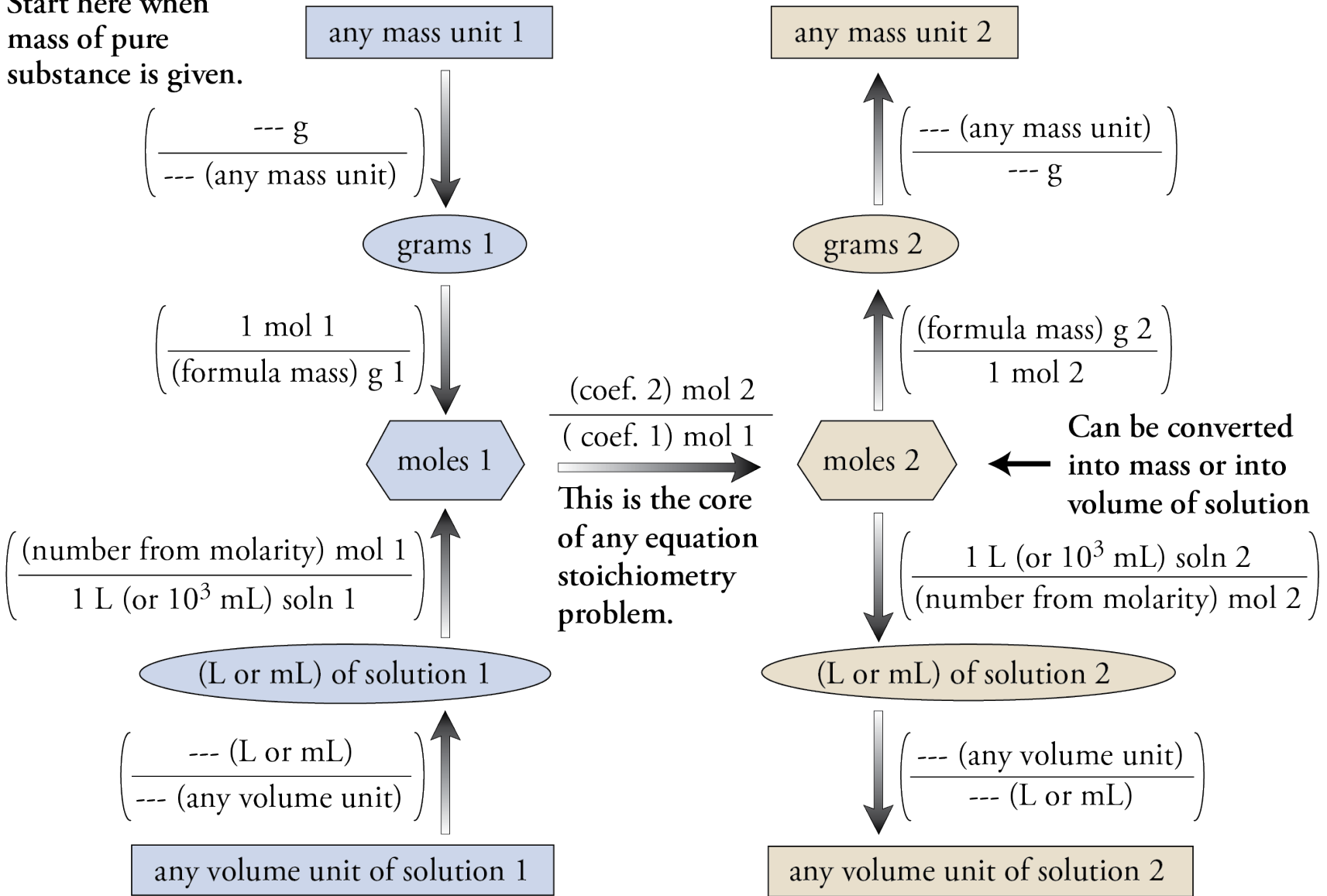
Calculating Molarity

- A silver perchlorate solution was made by dissolving 29.993 g of pure $AgClO_4$ in water and then diluting the mixture with additional water to achieve a total volume of 50.00 mL. What is the solution's molarity?

Molarity expressed with more specific units

Given amount of solute

Converts mass to moles

Converts the given volume unit into the desired volume unit

$$? \text{ M AgClO}_4 = \frac{? \text{ mol AgClO}_4}{1 \text{ L AgClO}_4 \text{ soln}} = \frac{29.993 \text{ g AgClO}_4}{50.00 \text{ mL AgClO}_4 \text{ soln}} \left(\frac{1 \text{ mol AgClO}_4}{207.3185 \text{ g AgClO}_4} \right) \left(\frac{10^3 \text{ mL}}{1 \text{ L}} \right)$$

Given amount of solution

$$= \frac{2.893 \text{ mol AgClO}_4}{1 \text{ L AgClO}_4 \text{ soln}} = \textbf{2.893 M AgClO}_4$$

Equation Stoichiometry

Start here when mass of pure substance is given.

any mass unit 1

$$\left(\frac{\text{--- g}}{\text{--- (any mass unit)}} \right)$$

grams 1

$$\left(\frac{\text{1 mol 1}}{\text{(formula mass) g 1}} \right)$$

moles 1

$$\frac{\text{(coef. 2) mol 2}}{\text{(coef. 1) mol 1}}$$

This is the core of any equation stoichiometry problem.

$$\left(\frac{\text{(number from molarity) mol 1}}{\text{1 L (or } 10^3 \text{ mL) soln 1}} \right)$$

(L or mL) of solution 1

$$\left(\frac{\text{--- (L or mL)}}{\text{--- (any volume unit)}} \right)$$

any volume unit of solution 1

Start here when volume of solution is given.

any mass unit 2

$$\left(\frac{\text{--- (any mass unit)}}{\text{--- g}} \right)$$

grams 2

$$\left(\frac{\text{(formula mass) g 2}}{\text{1 mol 2}} \right)$$

moles 2

Can be converted into mass or into volume of solution

$$\left(\frac{\text{1 L (or } 10^3 \text{ mL) soln 2}}{\text{(number from molarity) mol 2}} \right)$$

(L or mL) of solution 2

$$\left(\frac{\text{--- (any volume unit)}}{\text{--- (L or mL)}} \right)$$

any volume unit of solution 2

Equation Stoichiometry (2)

- **Tip-off -** The calculation calls for you to convert from amount of one substance to amount of another, both of which are involved in a chemical reaction.

- **General Steps**

1. If you are not given it, write and balance the chemical equation for the reaction.

2. Start your unit analysis in the usual way.

3. Convert from the units that you are given for substance 1 to moles of substance 1.

- For pure solids and liquids, this means converting mass to moles using the molar mass of the substance.

- Molarity can be used to convert from volume of solution to moles of solute.

Equation Stoichiometry (4)

4. Convert from moles of substance 1 to moles of substance 2, using the coefficients in the balanced equation.

5. Convert from moles of substance 2 to the desired units for substance 2.
   - For pure solids and liquids, this means converting moles to mass using the molar mass of substance 2.
   - Molarity can be used to convert from moles of solute to volume of solution.

Equation Stoichiometry (4)

6. If necessary, we convert from grams to the mass unit we want, or liters (or milliliters) to the volume unit we want.

7. Calculate your answer and report it with the correct significant figures (in scientific notation, if necessary) and unit.

Example 1

- How many milliliters of 6.00 M HNO_3 are necessary to neutralize the carbonate in 75.00 mL of 0.250 M Na_2CO_3?

$$\left(\frac{0.250 \text{ mol Na}_2\text{CO}_3}{10^3 \text{ mL Na}_2\text{CO}_3 \text{ soln}} \right) \qquad \left(\frac{10^3 \text{ mL HNO}_3 \text{ soln}}{6.00 \text{ mol HNO}_3} \right)$$

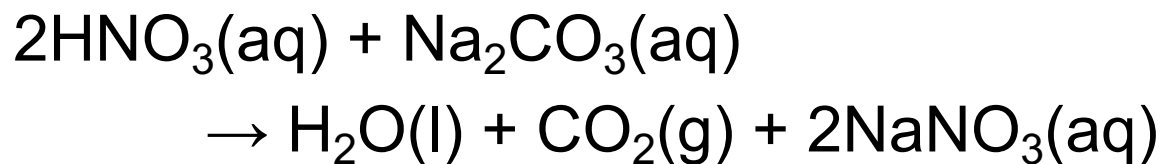| mL Na$_2$CO$_3$ soln | → | mol Na$_2$CO$_3$ | → | mol HNO$_3$ | → | mL HNO$_3$ soln |

Example 1

How many milliliters of 6.00 M HNO_3 are necessary to neutralize the carbonate in 75.00 mL of 0.250 M Na_2CO_3?

- Before we can do our calculation, we need to get a balanced equation.

- HNO_3 is a strong acid and Na_2CO_3 as a weak base, so we follow the steps described in a previous lesson for writing double displacement equations for acid-base reactions.

$$2HNO_3(aq) + Na_2CO_3(aq)$$
$$\rightarrow H_2O(l) + CO_2(g) + 2NaNO_3(aq)$$

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$$2HNO_3(aq) + Na_2CO_3(aq) \rightarrow H_2O(l) + CO_2(g) + 2NaNO_3(aq)$$

$$? \text{ mL HNO}_3 \text{ soln} = 75.00 \text{ mL Na}_2\text{CO}_3 \text{ soln} \left(\frac{}{\text{mL Na}_2\text{CO}_3 \text{ soln}} \right)$$

$$? \text{ mL HNO}_3 \text{ soln} = 75.00 \text{ mL Na}_2\text{CO}_3 \text{ soln} \left(\frac{0.250 \text{ mol Na}_2\text{CO}_3}{10^3 \text{ mL Na}_2\text{CO}_3 \text{ soln}} \right)$$

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$$? \text{ mL HNO}_3 \text{ soln} = 75.00 \text{ mL Na}_2\text{CO}_3 \text{ soln} \left(\frac{0.250 \text{ mol Na}_2\text{CO}_3}{10^3 \text{ mL Na}_2\text{CO}_3 \text{ soln}} \right) \left(\frac{2 \text{ mol HNO}_3}{1 \text{ mol Na}_2\text{CO}_3} \right) \left(\frac{10^3 \text{ mL HNO}_3 \text{ soln}}{6.00 \text{ mol HNO}_3} \right)$$

$$? \text{ mL HNO}_3 \text{ soln} = 75.00 \text{ mL Na}_2\text{CO}_3 \text{ soln} \left(\frac{0.250 \text{ mol Na}_2\text{CO}_3}{10^3 \text{ mL Na}_2\text{CO}_3 \text{ soln}} \right) \left(\frac{2 \text{ mol HNO}_3}{1 \text{ mol Na}_2\text{CO}_3} \right) \left(\frac{10^3 \text{ mL HNO}_3 \text{ soln}}{6.00 \text{ mol HNO}_3} \right)$$

$$= \textbf{6.25 mL HNO}_3 \textbf{ soln}$$

Coefficients from balanced equation convert moles of one substance into moles of another substance.

$$? \text{ mL HNO}_3 \text{ soln} = 75.00 \text{ mL Na}_2\text{CO}_3 \text{ soln} \left(\frac{0.250 \text{ mol Na}_2\text{CO}_3}{10^3 \text{ mL Na}_2\text{CO}_3 \text{ soln}} \right) \left(\frac{2 \text{ mol HNO}_3}{1 \text{ mol Na}_2\text{CO}_3} \right) \left(\frac{10^3 \text{ mL HNO}_3 \text{ soln}}{6.00 \text{ mol HNO}_3} \right)$$
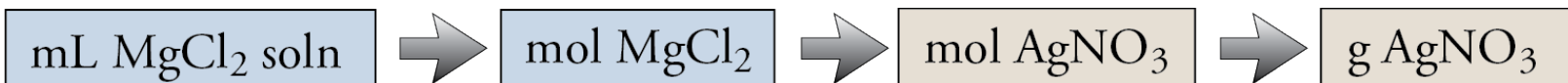
$$= \textbf{6.25 mL HNO}_3 \textbf{ soln}$$

Molarity as a conversion factor converts liters into moles.

Molarity as a conversion factor converts moles into liters.

Example 2

- What is the maximum number of grams of silver chloride that will precipitate from a solution made by mixing 25.00 mL of 0.050 M $MgCl_2$ with an excess of $AgNO_3$ solution?
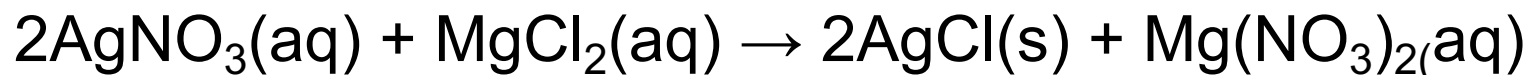
$$\left(\frac{0.050 \text{ mol } MgCl_2}{10^3 \text{ mL } MgCl_2 \text{ soln}} \right)$$

| mL $MgCl_2$ soln	→	mol $MgCl_2$	→	mol $AgNO_3$	→	g $AgNO_3$

Example 2

What is the maximum number of grams of silver chloride that will precipitate from a solution made by mixing 25.00 mL of 0.050 M $MgCl_2$ with an excess of $AgNO_3$ solution?

- Before we can do our calculation, we need to get a balanced equation.

- This is a precipitation reaction, so we follow the steps described in a previous lesson for writing double displacement equations for precipitation reactions.

$2AgNO_3(aq) + MgCl_2(aq) \rightarrow 2AgCl(s) + Mg(NO_3)_2(aq)$

Example 2

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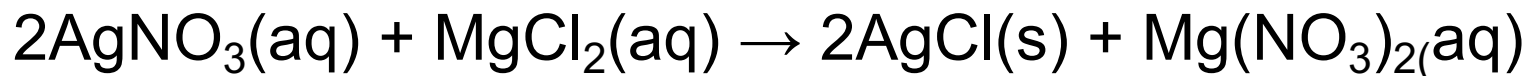
$$\text{g AgCl} = 25.00 \cancel{\text{ mL MgCl}_2 \text{ soln}} \left(\frac{}{\cancel{\text{mL MgCl}_2 \text{ soln}}} \right)$$

$$\text{g AgCl} = 25.00 \cancel{\text{ mL MgCl}_2 \text{ soln}} \left(\frac{0.050 \text{ mol MgCl}_2}{10^3 \cancel{\text{ mL MgCl}_2 \text{ soln}}} \right)$$

$$\text{g AgCl} = 25.00 \cancel{\text{ mL MgCl}_2 \text{ soln}} \left(\frac{0.050 \cancel{\text{ mol MgCl}_2}}{10^3 \cancel{\text{ mL MgCl}_2 \text{ soln}}} \right) \left(\frac{}{\cancel{\text{mol MgCl}_2}} \right)$$

$$\text{g AgCl} = 25.00 \cancel{\text{ mL MgCl}_2 \text{ soln}} \left(\frac{0.050 \cancel{\text{ mol MgCl}_2}}{10^3 \cancel{\text{ mL MgCl}_2 \text{ soln}}} \right) \left(\frac{2 \text{ mol AgCl}}{1 \cancel{\text{ mol MgCl}_2}} \right)$$

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$$\text{g AgCl} = 25.00 \ \cancel{\text{mL MgCl}_2 \text{ soln}} \left(\frac{0.050 \ \cancel{\text{mol MgCl}_2}}{10^3 \ \cancel{\text{mL MgCl}_2 \text{ soln}}} \right) \left(\frac{2 \ \cancel{\text{mol AgCl}}}{1 \ \cancel{\text{mol MgCl}_2}} \right) \left(\frac{143.3209 \ \text{g AgCl}}{1 \ \cancel{\text{mol AgCl}}} \right)$$

$$\text{g AgCl} = 25.00 \ \cancel{\text{mL MgCl}_2 \text{ soln}} \left(\frac{0.050 \ \cancel{\text{mol MgCl}_2}}{10^3 \ \cancel{\text{mL MgCl}_2 \text{ soln}}} \right) \left(\frac{2 \ \cancel{\text{mol AgCl}}}{1 \ \cancel{\text{mol MgCl}_2}} \right) \left(\frac{143.3209 \ \text{g AgCl}}{1 \ \cancel{\text{mol AgCl}}} \right)$$

$$= 0.36 \ \text{g AgCl}$$