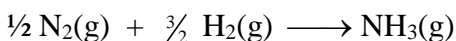


## Moles of Reaction and Limiting Reactant

Consider the gaseous reaction:  $\text{N}_2(\text{g}) + 3 \text{H}_2(\text{g}) \longrightarrow 2 \text{NH}_3(\text{g})$

The smallest amount of reaction possible is that one (1) molecule of  $\text{N}_2$  combines with three (3) molecules of  $\text{H}_2$  to produce two (2) molecules of  $\text{NH}_3$ . When this simple reaction involving individual molecules occurs  $6.022 \times 10^{23}$  times, it is said that **one mole of reaction** has occurred. In this case (according to the equation above) one mole of reaction is the combination of 1 mole of  $\text{N}_2$  with 3 moles of  $\text{H}_2$  to produce 2 moles of  $\text{NH}_3$ . If 2 moles of  $\text{N}_2$  combine with 6 moles of  $\text{H}_2$  to produce 4 moles  $\text{NH}_3$ , that would be two moles of reaction.

The moles of reaction depend upon how the equation is written. If the equation is written as:



Then one mole of reaction would produce 1 mole of  $\text{NH}_3$  from one-half mole of  $\text{N}_2$  and one and one-half moles of  $\text{H}_2$ . Essentially one mole of reaction means the equation as written occurs on the molecular level  $6.022 \times 10^{23}$  (1 mole) times.

Consider again the equation:  $\text{N}_2(\text{g}) + 3 \text{H}_2(\text{g}) \longrightarrow 2 \text{NH}_3(\text{g})$

To react 2 moles of  $\text{N}_2$  with 6 moles of  $\text{H}_2$  would produce 2 moles of reaction. Or 3 moles of  $\text{N}_2$  reacted with 9 moles of  $\text{H}_2$  will produce 3 moles of reaction. And so on. In each case **the moles of reaction can be calculated by dividing the amount of reactant by its coefficient in the equation**. For example,

$$9 \text{ moles H}_2 = ? \text{ mol reaction}$$

$$9 \text{ mol H}_2 = 9 \text{ mol H}_2 \times \frac{1 \text{ mol reaction}}{3 \text{ mol H}_2} = 3 \text{ mol reaction}$$

Then the amount of product is determined by multiplying the coefficient of the product times the mole of reaction.

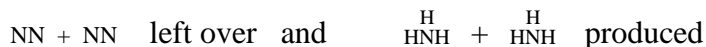
$$3 \text{ mol reaction} = ? \text{ mol NH}_3$$

$$3 \text{ mol reaction} = 3 \text{ mol reaction} \times \frac{2 \text{ mol NH}_3}{1 \text{ mol reaction}} = 6 \text{ mol NH}_3$$

Start the reaction with just 3 molecules of  $\text{N}_2$  and 3 molecules of  $\text{H}_2$ .



One can see that 1 molecule of  $\text{N}_2$  will combine with 3 molecules of  $\text{H}_2$  to produce 2 molecules of  $\text{NH}_3$ .



The  $\text{H}_2$  will be all used up and there will be 2 molecules of  $\text{N}_2$  left over.  $\text{N}_2$  is said to be **in excess** and  $\text{H}_2$  is said to be **the limiting reactant**, because when one reactant runs out the reaction must stop. The extent of the reaction is limited by the reactant that disappears first.

Still using the equation:  $\text{N}_2(\text{g}) + 3 \text{H}_2(\text{g}) \longrightarrow 2 \text{NH}_3(\text{g})$

We need to be able to determine the limiting reactant when the reaction is scaled up to moles of reactants.

**Problem 1.** Starting with 3 moles of  $N_2$  ( $3 \times 6.022 \times 10^{23}$  molecules) and 3 moles of  $H_2$ , determine which is the limiting reactant, and determine the maximum moles of  $NH_3$  that can be produced. Calculate the moles of reaction for each reactant:

$$3 \text{ mole } N_2 \times \frac{1 \text{ mol rxn}}{1 \text{ mol } N_2} = 3 \text{ mol rxn} \quad \text{and} \quad 3 \text{ mole } H_2 \times \frac{1 \text{ mol rxn}}{3 \text{ mol } H_2} = 1 \text{ mol rxn}$$

**The reactant that provides the least moles of reaction is the limiting reactant.** All reactants that provide more moles of reaction than the limiting reactant are in excess. When the limiting reactant is used up, there will be no more reaction. So **moles of reaction is determined by the limiting reactant.** In this case 1 mol rxn (from  $H_2$ ) < 3 mol rxn (from  $N_2$ ), so the  $H_2$  limits the reaction to 1 mole of reaction. The amount of product depends upon the (limiting) moles of reaction.

$$1 \text{ mol rxn} = ? \text{ mol } NH_3 \quad 1 \text{ mol rxn} = 1 \text{ mol rxn} \times \frac{2 \text{ mol } NH_3}{1 \text{ mol rxn}} = 2 \text{ mol } NH_3$$

It is a little more complicated if reactant masses are given (instead of moles).

**Problem 2.** Starting with 100.0 g  $N_2$  and 30.0 g  $H_2$  determine the theoretical yield of  $NH_3$  (maximum grams that can be produced) by the reaction:  $N_2(g) + 3 H_2(g) \longrightarrow 2 NH_3(g)$

Solution: First determine the limiting reactant. **To determine the limiting reactant, calculate moles of reaction for each reactant.** The reactant with smallest moles of reaction is limiting.

$$? \text{ mol rxn} = 100. \text{ g } N_2 \times \frac{1 \text{ mol } N_2}{28.01 \text{ g } N_2} \times \frac{1 \text{ mol rxn}}{1 \text{ mol } N_2} = 3.57 \text{ mol rxn}$$

$$? \text{ mol rxn} = 30.0 \text{ g } H_2 \times \frac{1 \text{ mol } H_2}{2.016 \text{ g } H_2} \times \frac{1 \text{ mol rxn}}{3 \text{ mol } H_2} = 4.96 \text{ mol rxn} > 3.57 \text{ mol so } N_2 \text{ limiting}$$

$$? \text{ g } NH_3 = 3.57 \text{ mol rxn} \times \frac{2 \text{ mol } NH_3}{1 \text{ mol rxn}} \times \frac{17.03 \text{ g } NH_3}{1 \text{ mol } NH_3} = 121.6 \text{ g } NH_3 \text{ produced (= theoretical yield)}$$

The amount of  $H_2$  in excess (or left over) can be determined by subtracting the amount of  $H_2$  used up from the initial amount of  $H_2$ . The amount used up depends upon the moles of reaction.

$$? \text{ g } H_2 \text{ used} = 3.57 \text{ mol rxn} \times \frac{3 \text{ mol } H_2}{1 \text{ mol rxn}} \times \frac{2.016 \text{ g } H_2}{1 \text{ mol } H_2} = 21.6 \text{ g } H_2 \text{ used}$$

$$\text{so } 30.0 \text{ g } H_2 \text{ starting} - 21.6 \text{ g } H_2 \text{ used} = 8.4 \text{ g } H_2 \text{ remaining}$$

**Problem 3.** 120.0 g  $Br_2$  are mixed with 120.0 g  $F_2$  and reacted according to the equation,  $Br_2(g) + 5 F_2(g) \longrightarrow 2 BrF_5(g)$ , until one of the reactants is used up. Calculate the maximum grams of  $BrF_5$  that can be produced and which reactant and how many grams will be left over.

**Problem 4.** 200.0 g  $Cl_2$  react with 300.0 g  $Fe_2O_3$  according to the equation:  $6 Cl_2(g) + 2 Fe_2O_3(s) \longrightarrow 4 FeCl_3(s) + 3 O_2(g)$ , until one react is used up. Determine the theoretical yield of  $FeCl_3(s)$ , and which reactant and how grams will remain.

**Problem 5.** 94.0 g  $CaO$  is reacted with 94.0 g  $C(s)$  according to the equation:  $2 CaO(s) + 5 C(s) \longrightarrow 2 CaC_2(s) + 5 CO_2(g)$ , until one of the reactants is used up. Determine the theoretical yield of  $CaC_2$ , and which reactant and how many grams will remain.

Answers:

3. ( $Br_2$ ) mol rxn 0.751 > **0.632 mol rxn** ( $F_2$ )  $\Rightarrow$  221. g  $BrF_5$ ; 101.0 g  $Br_2$  used  $\Rightarrow$  19.0 g remain

4. ( $Cl_2$ ) **mol rxn 0.470** < 0.939 mol rxn ( $Fe_2O_3$ )  $\Rightarrow$  304.9 g  $FeCl_3$ ; 150.1 g  $Fe_2O_3$  used  $\Rightarrow$  149.9 g left

5. ( $CaO$ ) **mol rxn 0.838** < 1.567 mol rxn ( $C$ )  $\Rightarrow$  107.4 g  $CaC_2$ ; 50.3 g  $C$  used  $\Rightarrow$  43.7 g  $C$  left

Solutions.

$$3. \quad 120.0 \text{ g Br}_2 \times \frac{1 \text{ mol Br}_2}{159.8 \text{ g Br}_2} = 0.7509 \text{ mol Br}_2 \times \frac{1 \text{ mol rxn}}{1 \text{ mol Br}_2} = 0.7509 \text{ mol rxn}$$

$$120.0 \text{ g F}_2 \times \frac{1 \text{ mol F}_2}{38.00 \text{ g F}_2} = 3.158 \text{ mol F}_2 \times \frac{1 \text{ mol rxn}}{5 \text{ mol F}_2} = 0.6316 \text{ mol rxn}$$

$$0.6316 \text{ mol rxn} \times \frac{2 \text{ mol BrF}_3}{1 \text{ mol rxn}} \times \frac{174.9 \text{ g BrF}_3}{1 \text{ mol BrF}_3} = 220.9 \text{ g BrF}_3$$

$$0.6316 \text{ mol rxn} \times \frac{1 \text{ mol Br}_2}{1 \text{ mol rxn}} \times \frac{159.8 \text{ g Br}_2}{1 \text{ mol Br}_2} = 100.9 \text{ g Br}_2 \text{ used}$$

$$\text{so } 120.0 \text{ g Br}_2 - 100.9 \text{ g Br}_2 = 19.1 \text{ g Br}_2 \text{ left}$$

$$4. \quad 200.0 \text{ g Cl}_2 \times \frac{1 \text{ mol Cl}_2}{70.91 \text{ g Cl}_2} = 2.820 \text{ mol Cl}_2 \times \frac{1 \text{ mol rxn}}{6 \text{ mol Cl}_2} = 0.4701 \text{ mol rxn}$$

$$300.0 \text{ g Fe}_2\text{O}_3 \times \frac{1 \text{ mol Fe}_2\text{O}_3}{159.6 \text{ g Fe}_2\text{O}_3} = 1.880 \text{ mol Fe}_2\text{O}_3 \times \frac{1 \text{ mol rxn}}{2 \text{ mol Fe}_2\text{O}_3} = 0.9398 \text{ mol rxn}$$

$$0.4701 \text{ mol rxn} \times \frac{4 \text{ mol FeCl}_3}{1 \text{ mol rxn}} \times \frac{162.2 \text{ g FeCl}_3}{1 \text{ mol FeCl}_3} = 305.0 \text{ g FeCl}_3$$

$$\text{mol rxn excess for Fe}_2\text{O}_3 = 0.9398 - 0.4701 =$$

$$0.4697 \text{ mol rxn} \times \frac{2 \text{ mol FeO}}{1 \text{ mol rxn}} \times \frac{159.6 \text{ g Fe}_2\text{O}_3}{1 \text{ mol Fe}_2\text{O}_3} = 149.9 \text{ g Fe}_2\text{O}_3$$

Or once **moles** of reactants are calculated one can set up the problem as follows:

|                                |  |                                    |
|--------------------------------|--|------------------------------------|
|                                | $6 \text{ Cl}_2 + 2 \text{ Fe}_2\text{O}_3 \longrightarrow 4 \text{ FeCl}_3 + 3 \text{ O}_2$ |                                    |
|                                | 0.4701      0.9398   |                                    |
| starting quantities (in moles) | 2.820      1.880      0      0   | moles of rxn = moles / coefficient |
| change line                    | -2.820      -0.9402      +1.880      +1.410  | = coefficient $\times$ 0.4701      |
| Final quantities (in moles)    | 0      0.9398      1.880      1.410  |                                    |

$$1.880 \text{ mol FeCl}_3 \times \frac{162.2 \text{ g FeCl}_3}{1 \text{ mol FeCl}_3} = 304.9 \text{ g FeCl}_3 \text{ produced}$$

$$0.9398 \text{ mol Fe}_2\text{O}_3 \times \frac{159.6 \text{ g Fe}_2\text{O}_3}{1 \text{ mol Fe}_2\text{O}_3} = 150.0 \text{ g Fe}_2\text{O}_3 \text{ remaining}$$

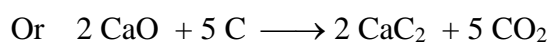
$$5. \quad 94.0 \text{ g CaO} \times \frac{1 \text{ mol CaO}}{56.08 \text{ g CaO}} = 1.676 \text{ mol CaO} \times \frac{1 \text{ mol rxn}}{2 \text{ mol CaO}} = 0.8381 \text{ mol rxn}$$

$$94.0 \text{ g Ca} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 7.827 \text{ mol C} \times \frac{1 \text{ mol rxn}}{5 \text{ mol C}} = 1.565 \text{ mol rxn}$$

$$0.8381 \text{ mol rxn} \times \frac{2 \text{ mol CaC}_2}{1 \text{ mol rxn}} \times \frac{64.10 \text{ g CaC}_2}{1 \text{ mol CaC}_2} = 107.4 \text{ g CaC}_2$$

$$0.8381 \text{ mol rxn} \times \frac{5 \text{ mol C}}{1 \text{ mol rxn}} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 50.3 \text{ g C used}$$

$$\text{so } 94.0 \text{ g C} - 50.3 \text{ g C} = 43.7 \text{ g C left}$$



|        |        |         |        |  |
|--------|--------|---------|--------|--|
| 0.8381 | 1.565  |         |        |  |
| 1.676  | 7.827  | 0       | 0      |  |
| -1.676 | -4.191 | +1.676  | +4.191 |  |
| 0.0    | 3.636  | + 1.676 | +4.191 |  |

= moles / coefficient = mol rxn (0.8381 is limiting)

= moles starting

= moles of change = coefficient  $\times$  limiting mol rxn (0.8381)

= final moles

$$\text{so } 1.676 \text{ mol CaC}_2 \times \frac{64.10 \text{ g CaC}_2}{1 \text{ mol CaC}_2} = 107.4 \text{ g CaC}_2 \text{ produced}$$

$$\text{and } 3.636 \text{ mol C} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 43.7 \text{ g C left}$$