Stoichiometry

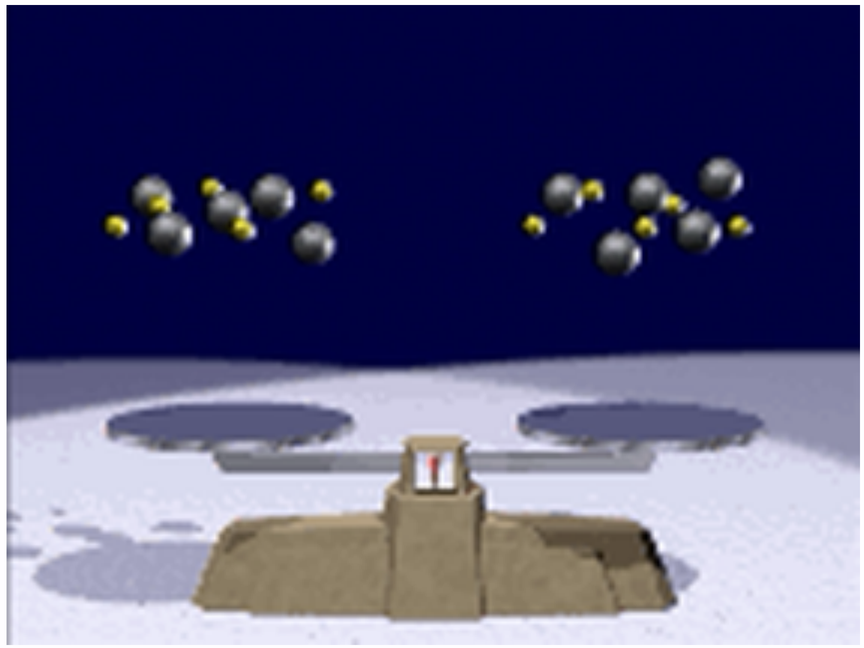
Dr. Ron Rusay

Chemical Stoichiometry

- *Stoichiometry is the study of mass in chemical reactions. It deals with both reactants and products.*
- *It quantitatively and empirically relates the behavior of atoms and molecules in a balanced chemical equation to observable chemical change and measurable mass effects.*
- *It accounts for mass and the conservation of mass, just as the conservation of atoms in a balanced chemical equation.*

Chemical Reactions

Atoms, Mass & Balance: eg. Zn(s) + S(s) $\longrightarrow$



Stoichiometry

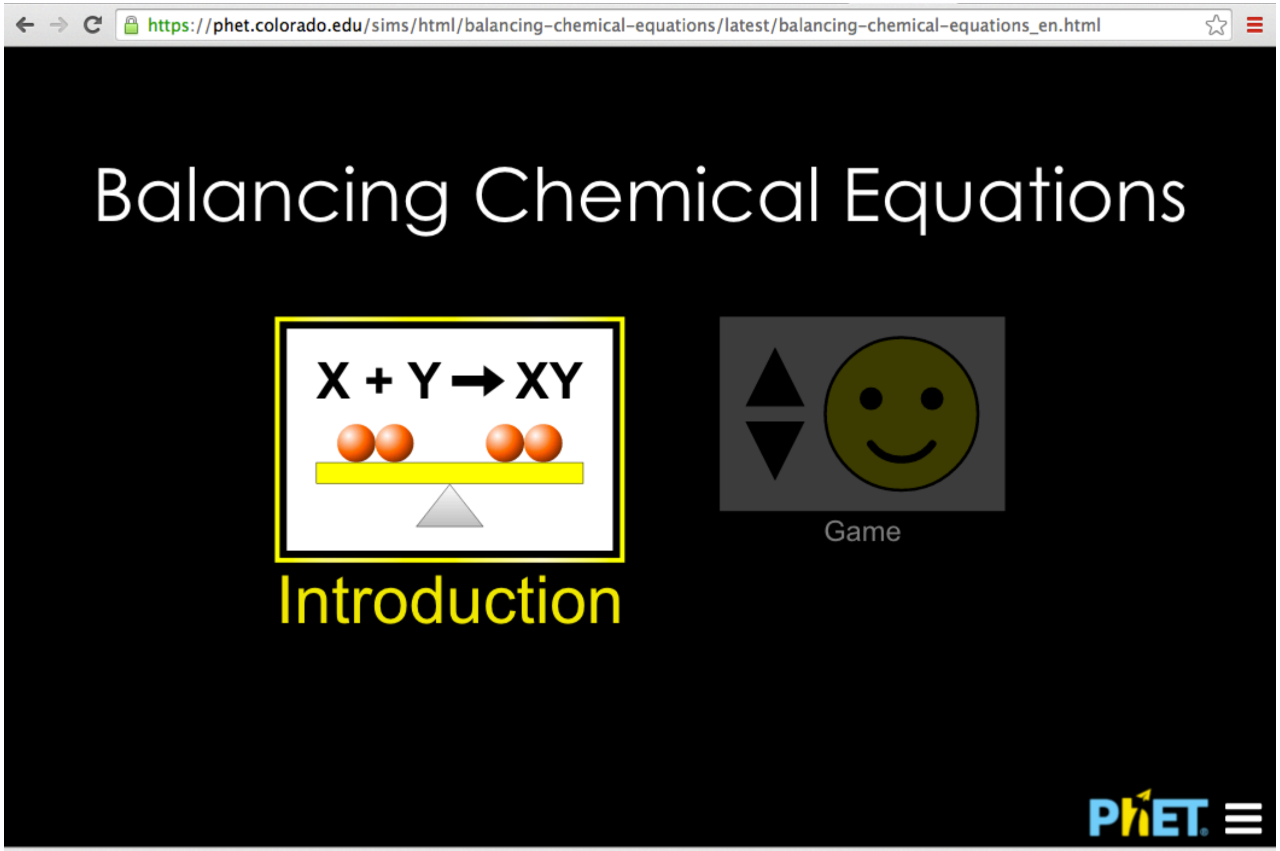
Must begin with a correctly balanced equation:

$$\_\ C_2H_5OH + \_\ O_2 \rightarrow \_\ CO_2 + \_\ H_2O$$

Reactants *Products*

- $C=2; H=5+1=6; O=2+1$ $C=1; H=2; O=2+1$
- $\underline{1}\ C_2H_5OH + \underline{3}\ O_2 \rightarrow \underline{2}\ CO_2 + \underline{3}\ H_2O$

https://phet.colorado.edu/sims/html/balancing-chemical-equations/latest/balancing-chemical-equations_en.html



Chemical Equation

$$C_2H_5OH + 3\,O_2 \rightarrow 2\,CO_2 + 3\,H_2O$$

The balanced equation can be completely stated as:

- *1 mole of ethanol reacts with 3 moles of oxygen to produce 2 moles of carbon dioxide and 3 moles of water.*

Chemical Equation

All Balanced Equations relate on a molar mass basis. For example the combustion of octane:

$$\mathbf{2}\ C_8H_{18(l)} + \mathbf{25}\ O_{2(g)} \longrightarrow \mathbf{16}\ CO_{2(g)} + \mathbf{18}\ H_2O_{(l)}$$

2 ***moles*** *of octane react with* ***25 moles*** *of oxygen to produce* ***16 moles*** *of carbon dioxide and* ***18 moles*** *of water.*

The Chemical Equation: Mole & Masses

$$C_2H_5OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$$

- 46g (1 mole) of ethanol reacts with 3 moles of oxygen (96g) to produce 2 moles of carbon dioxide and 3 moles of water.
- How many grams of carbon dioxide and water are respectively produced from 46g (1 mole) of ethanol ?

2 mol x 44 g/mol = 88g 3 mol x 18 g/mol = 54 g

The Chemical Equation: Moles & Masses

- $C_2H_5OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$

ð *How many grams of oxygen are needed to react with 15.3g of ethanol in a 12oz. beer ?*

$$15.3g_{ethanol} \times mol_{ethanol}/46.0g_{ethanol} = 0.333mol_{ethanol}$$

$$0.333mol_{ethanol} \times 3mol_{oxygen} / 1mol_{ethanol} = 0.999mol_{oxygen}$$

$$32.0g_{oxygen}/mol_{oxygen} \times 0.999mol_{oxygen} = 32.0g_{oxygen}$$

NOTE: It takes approximately 1 hour for the biologically equivalent amount of oxygen available from cytochrome p450 to consume the alcohol in a human in 1 beer to a level below the legal limit of 0.08%.

Chemical Stoichiometry

- *Epsom salt (magnesium sulfate heptahydrate) is one of five possible hydrates: mono-, di-, tri-, hexa-, or hepta- hydrate.*
- *How can stoichiometry be used to determine, which hydrate is present in a pure unknown sample, by heating the sample in a kitchen oven at 400 ^{o} C for 45 minutes?*

$$MgSO_4 \cdot x\, H_2O_{(s)} \longrightarrow MgSO_{4\ (s)} + x\, H_2O_{\ (g)}$$

Refer to % Hydrate Lab Experiment.

Mass Calculations

All Balanced Equations relate on a molar and mass basis. For the combustion of octane:

$$\mathbf{2}\ C_8H_{18(l)} + \mathbf{25}\ O_{2(g)} \longrightarrow \mathbf{16}\ CO_{2(g)} + \mathbf{18}\ H_2O_{(l)}$$

*228 g of octane **(2 moles)*** will react with 800 g of oxygen **(25 moles)** to produce **(16 moles)** 704 g of carbon dioxide and **(18 moles)** 324 g of water.*

****(2 moles octane x 114 g/mol = 228 g)***

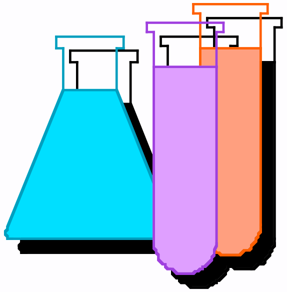
Mass Calculations: Reactants $\longleftrightarrow$ Products

Chemically Relate:

Something (S) $\longrightarrow$ Another Thing (AT)

Mass (S) $\longrightarrow$ Mass (AT)

grams (S) $\longrightarrow$ grams (AT)



Mass Calculations: Reactants $\longleftrightarrow$ Products

1. *Balance the chemical equation.*
2. *Convert mass of reactant or product to moles.*
3. *Identify mole ratios in balanced equation:*
   They serve as the "Gatekeeper".
4. *Calculate moles of desired product or reactant.*
5. *Convert moles to grams.*

Mass Calculations: Reactants ⟷ Products

grams (S) ⟶ grams (AT)

Avogadro's Number
Atoms
Molecules
Stoichiometry

grams (S)	1 mol (S)	?	grams (AT) (Molecular Weight)	= grams (AT)
	grams (S) (Molecular Weight)	?	1 mol (AT)	

"Gatekeeper"

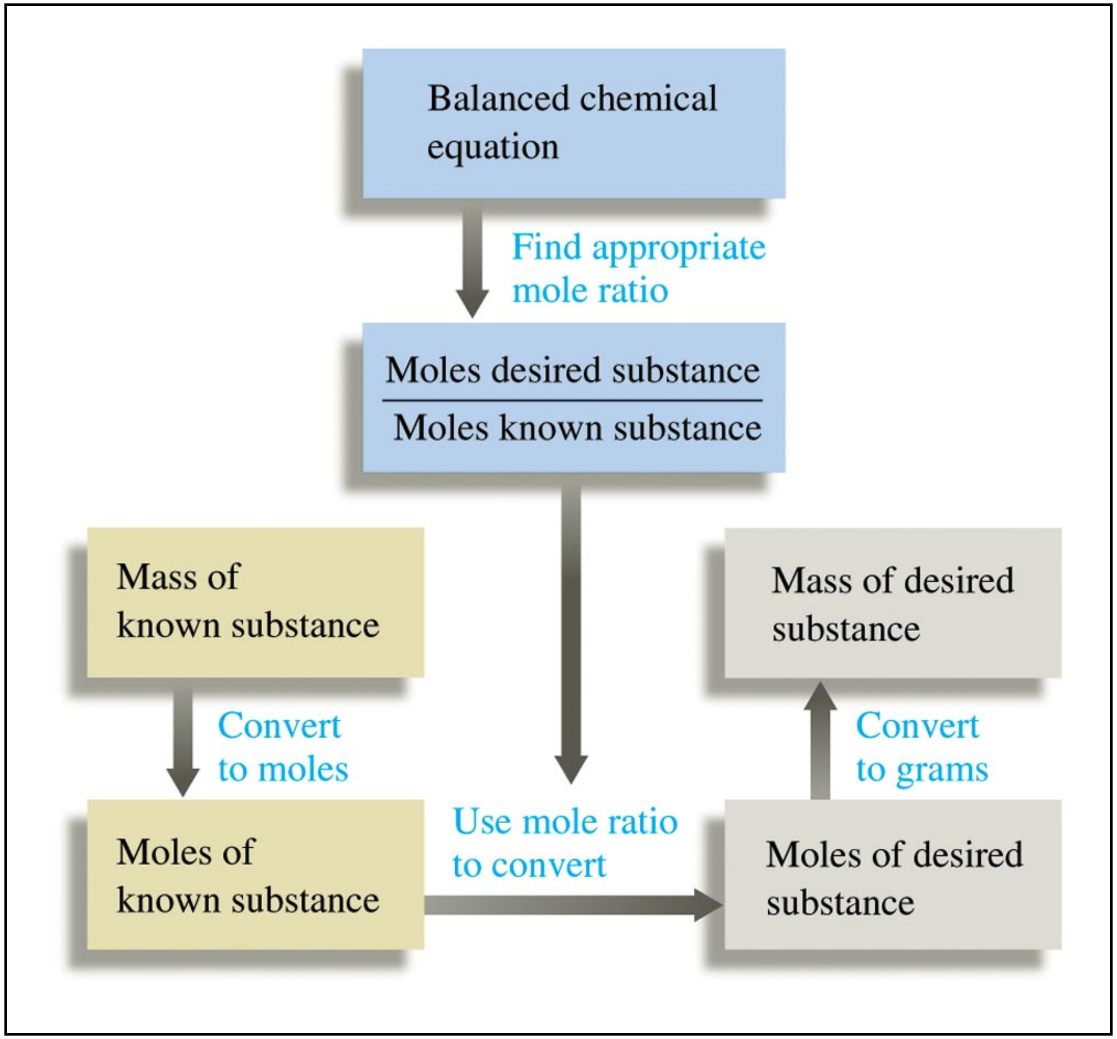
QUESTION

The fuel in small portable lighters is butane (C_4H_{10}). After using a lighter for a few minutes, 1.0 gram of fuel was used. How many moles of carbon dioxide would it produce?

A. 58 moles
B. 0.017 moles
C. 1.7×10^{-24} moles
D. 0.068 moles

$$? \, C_4H_{10}(g) + ? \, O_2(g) \rightarrow ? \, CO_2(g) + ? \, H_2O(g)$$

Mass Calculations: Reactants ⟷ Products



QUESTION

The fuel in small portable lighters is butane (C_4H_{10}). After using a lighter for a few minutes, 1.0 gram (0.017 moles) of fuel was used. How many grams of carbon dioxide would it produce?

$$2\ C_4H_{10}(g) + 13\ O_2(g) \rightarrow 8\ CO_2(g) + 10\ H_2O(g)$$

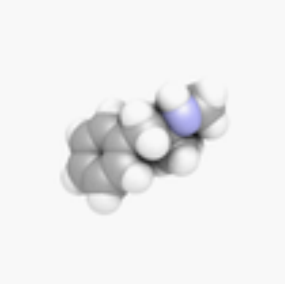
How many grams of carbon dioxide would this produce?

A.) 750 mg

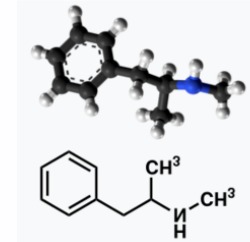
B.) 6.0 g

C) 1.5 g

D.) 3.0 g



Percent Yield



- *In synthesis as in any experimentation, it is very difficult and at most times impossible to be perfect. Therefore the actual yield (g) is measured and compared to the theoretical calculated yield (g). This is the percent yield:*

- *% Yield = actual (g) / theoretical (g) x 100*

Some DVC students may report percent yields greater than 100% in their first synthesis experiment. Hmmm?....... Why is this not possible?

Theoretical (Yield) Mass Calculations
Reactant → ***Product***

grams (Reactant) → **grams (Product)**

Moles

Molar Mass

grams (R)	1 mol (R)	? mol (P)	grams (P)	
	grams (R)	? mol (R)	1 mol (P)	= ? grams (P)
	(Divide) by Molar Mass (R)	***"Gatekeepers" from Balanced reaction***	***(Multiply)*** by Molar Mass (P)	

Theoretical (Yield) Mass Calculation

$$1\ C_{20}H_{24}N_2O_{(s)} + H_{2\,(g)} \rightarrow 1\ C_{20}H_{26}N_2O_{(s)}$$

Ibogaine

3.03 grams ($C_{20}H_{24}N_2O$. **Reactant**) → **?** grams ($C_{20}H_{26}N_2O$ **Product**)

Ibogaine

308.4 g mol^{-1}

Moles

Molar Mass

310.4 g mol^{-1}

$$\frac{3.03\ \text{grams (R } C_{20}H_{24}N_2O)}{} \times \frac{1\ \text{mol (R)}}{308.4\ \text{Grams (R } C_{20}H_{24}N_2O)} \times \frac{1\ \text{mol (P)}}{1\ \text{mol (R)}} \times \frac{310.4\ \text{grams (P } C_{20}H_{26}N_2O)}{1\ \text{mol (P)}} = ?\ \text{grams (P)}$$

3.05

(Divide)

by Molar Mass (R $C_{20}H_{24}N_2O$)

"Gatekeepers" from Balanced reaction

(Multiply)

by Molar Mass (P $C_{20}H_{26}N_2O$)

QUESTION

- *A synthetic hydrogenation reaction produced 2.85g of Ibogaine, $C_{20}H_{26}N_2O$, a natural product with strong promise in treating heroin addiction (at least in Europe), the calculated theoretical yield was 3.05g, what is the % yield?*

A) 6.6% *B) 80.3%* *C) 93.4%* *D) 107%*