Chemical Reactions

- When atoms or molecules combine or break apart, we describe that process with a chemical equation:

$C + O_2 \rightarrow CO_2$	formation of carbon dioxide
$CH_4 + O_2 \rightarrow CO_2 + H_2O$	combustion of methane
$H_2O(\lambda) \rightarrow H^+(aq) + OH^-(aq)$	dissociation of water

Chemical Reactions

- A chemical equation has reactants and products

$C + O_2$	$\rightarrow$	CO_2
reactants		products

- Reactants always appear on the left side of the equation
- Products always appear on the right side of the equation
- Reactants and products are separated by an arrow indicating the direction of the reaction

Chemical Reactions

- A chemical equation must be "balanced"
  - The number of atoms of each element must be the same for both reactants and products

Example: $CH_4 + O_2 \rightarrow CO_2 + H_2O$

As written, we have the following atoms:

element	reactants	products
carbon	1	1
hydrogen	4	2
oxygen	2	3

Balancing Chemical Equations

- Process for balancing chemical equations:

1. Determine correct chemical formulas of all reactants and products
2. Start with "heavier" atoms—balance number of these on reactant and product sides of equation
3. If elements appear in equation as either reactants or products, balance these last
4. Electrical charge must be balanced

Balancing Chemical Reactions

Example: $CH_4 + O_2 \rightarrow CO_2 + H_2O$

- C atom is balanced as written
- Reactants have 4 H's, products only 2 H's: multiply H_2O by 2 to balance H atoms
  $CH_4 + O_2 \rightarrow CO_2 + 2\ H_2O$
- Reactants have 2 O's, products 4 O's: multiply O_2 by 2 to balance O atoms
  $CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$
- Equation is now balanced

Balancing Chemical Reactions

Example: $H_2(g) + O_2(g) \rightarrow H_2O(\lambda)$

- Is reaction balanced?
- Reactants have 2 O's, products only 1 O: multiply H_2O by 2 to balance O atoms
  $H_2(g) + O_2(g) \rightarrow 2\ H_2O(\lambda)$
- Reactants have 2 H's, products 4 H's: multiply H_2 by 2 to balance H atoms
  $2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(\lambda)$
- Equation is now balanced

Balancing Chemical Reactions

Example: $Fe(s) + O_2(g) \rightarrow Fe_2O_3(s)$

- Is reaction balanced?
- Iron: multiply reactant Fe by 2

  $2\ Fe(s) + O_2(g) \rightarrow Fe_2O_3(s)$
- Oxygen: multiply reactant O_2 by 3/2

  $2\ Fe(s) + 3/2\ O_2(g) \rightarrow Fe_2O_3(s)$
- We usually don't use fractional stoichiometric coefficients, so we multiply all of them by 2

  $4\ Fe(s) + 3\ O_2(g) \rightarrow 2\ Fe_2O_3(s)$

Balancing Chemical Reactions

Example: $H_2(g) + N_2(g) \rightarrow NH_3(g)$

- Is reaction balanced?
- Nitrogen: multiply product by 2

  $H_2(g) + N_2(g) \rightarrow 2\ NH_3(g)$
- Hydrogen: multiply reactant by 3

  $3\ H_2(g) + N_2(g) \rightarrow 2\ NH_3(g)$

Balancing Chemical Reactions

Example: $C_3H_8(g) + O_2(g) \rightarrow CO_2(g) + H_2O(\lambda)$

- Is reaction balanced?
- Carbon: multiply product by 3

  $C_3H_8(g) + O_2(g) \rightarrow 3\ CO_2(g) + H_2O(\lambda)$
- Hydrogen: multiply product by 4

  $C_3H_8(g) + O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(\lambda)$
- Oxygen: multiply reactant by 5

  $C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(\lambda)$

Balanced Chemical Equations

Examples: Reaction of ammonium perchlorate with aluminum

$NH_4ClO_4(s) + Al(s) \rightarrow Al_2O_3(s) + N_2(g) + HCl(g) + H_2O(g)$

- Nitrogen: multiply reactant by 2

  $2\ NH_4ClO_4(s) + Al(s)$

  $\rightarrow Al_2O_3(s) + N_2(g) + HCl(g) + H_2O(g)$
- Chlorine: multiply product by 2

  $2\ NH_4ClO_4(s) + Al(s)$

  $\rightarrow Al_2O_3(s) + N_2(g) + 2\ HCl(g) + H_2O(g)$

Balanced Chemical Equations

Examples: Reaction of ammonium perchlorate with aluminum

$NH_4ClO_4(s) + Al(s) \rightarrow Al_2O_3(s) + N_2(g) + HCl(g) + H_2O(g)$

- Hydrogen: multiply product by 3

  $2\ NH_4ClO_4(s) + Al(s)$

  $\rightarrow Al_2O_3(s) + N_2(g) + 2\ HCl(g) + 3\ H_2O(g)$

- Oxygen: multiply product by 5/3

  $2\ NH_4ClO_4(s) + Al(s)$

  $\rightarrow 5/3\ Al_2O_3(s) + N_2(g) + 2\ HCl(g) + 3\ H_2O(g)$

Balanced Chemical Equations

Examples: Reaction of ammonium perchlorate with aluminum

$NH_4ClO_4(s) + Al(s) \rightarrow Al_2O_3(s) + N_2(g) + HCl(g) + H_2O(g)$

- Aluminum: multiply reactant by 10/3

  $2\ NH_4ClO_4(s) + 10/3\ Al(s)$

  $\rightarrow 5/3\ Al_2O_3(s) + N_2(g) + 2\ HCl(g) + 3\ H_2O(g)$

- Remove fractional coefficients (multiply by 3):

  $6\ NH_4ClO_4(s) + 10\ Al(s)$

  $\rightarrow 5\ Al_2O_3(s) + 3\ N_2(g) + 6\ HCl(g) + 9\ H_2O(g)$

Balanced Chemical Equations

Examples:

$Mg(s) + H_3O^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g) + H_2O(\lambda)$

- As written, the only element out of balance is the hydrogen—balance H first: multiply both H_3O^+ and H_2O by 2

$\boxed{Mg(s) + 2\ H_3O^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g) + 2\ H_2O(\lambda)}$

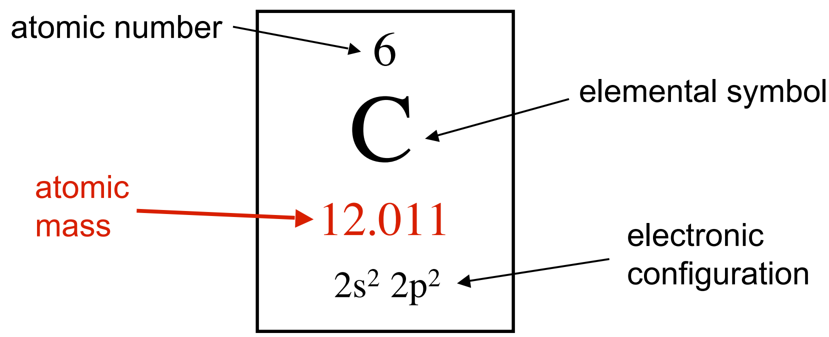
- Check charge balance:
  - left-hand side has total charge of +2 (2 * 1+ charge on hydronium ion)
  - Right-hand side has total charge of +2 (2+ charge on Mg ion)

The Mole

- The mole (a chemical unit, not a burrowing animal or reality-based TV series) is defined as the number of atoms in exactly 12 g of carbon-12
- 1 mole = 6.022×10^{23} atoms
- The mole is simply a unit of measure just like a dozen
- It is useful to denote very large numbers of chemical species
- $6.022 \times 10^{23}\ mol^{-1}$ is called Avagadro's Number

Molecular Weight (Formula Mass)

- *Atomic mass* of an element listed in the Periodic Table is the mass of one mole of the naturally occurring element.



Molecular Weight (Formula Mass)

- *Molecular weight* or *formula mass* of a molecule is the sum of the atomic masses of all atoms comprising that molecule.

  H_2:

  1 mol H = 1.0079 g

  2 mol H = 1 mol H_2

$$\frac{2\ \cancel{\text{mol H}}}{1\ \text{mol } H_2} \times \frac{1.0079\ \text{g}}{1\ \cancel{\text{mol H}}} = 2.0158\ \text{g/mol } H_2$$

Molecular Weight (Formula Mass)

Examples: H_2O

hydrogen:	2 x 1.008 g/mol	= 2.016 g/mol
oxygen:	1 x 15.999 g/mol	= 15.999 g/mol
molecular weight		= 18.015 g/mol

Molecular Weight

C_2H_6: 1 mol H = 1.0079 g
1 mol C = 12.011 g

(2 mol C) (12.011 g /mol C) = 24.022 g
(6 mol H) (1.0079 g/mol H) = 6.0474 g

1 mol C_2H_6 (molar mass) = 30.069 g

Molecular Weight

$Na_2Ni(NH_3)_6$:

(2 mol Na)(22.990 g/mol Na)	=	45.980 g
(1 mol Ni)(58.693 g /mol Ni)	=	58.693 g
(6 mol N)(14.007 g/mol N)	=	84.042 g
(18 mol H)(1.0079 g/mol H)	=	18.1422 g
1 mol $Na_2Ni(NH_3)_6$	=	206.827 g

Mass-Mole Conversions

- We can use the mass of an element to determine how many moles of element we have, or *vice versa*

<u>Example:</u> Which has more molecules: 20 g of O_2 or 20 g of H_2?

1. Determine *molecular weight (mass)* of each molecule:

   O_2: 2 x atomic mass of O = 2 x 15.999 g/mol
   = 31.998 g/mol

   H_2: 2 x atomic mass of H = 2 x 1.008 g/mol
   = 2.016 g/mol

Mass-Mole Conversions

Example: Which has more molecules: 20 g of O_2 or 20 g of H_2?

2. Determine mole of each element from given mass:
   - O_2: (20 g)/(31.998 g/mol) = 0.625 mol O_2
   - H_2: (20 g)/(2.016 g/mol) = 9.92 mol H_2

- Even though there are equal masses of each element, there are a lot more hydrogen molecules than oxygen molecules because H_2 weighs a lot less than O_2

Mole-Mass Conversions

- Using molar mass, we can now calculate the number of moles or the mass of any compound if we know the other quantity.

  How many moles in 6.358 g H_2?

$$6.358\ \cancel{g}\ H_2 \ \frac{(1 \text{ mol } H_2)}{(2.0158\ \cancel{g})} = 3.154 \text{ mol } H_2$$

Mass-Mole Conversions

<u>Examples:</u> NH_4NO_3 ammonium nitrate

hydrogen:	4 x 1.01 g/mol	= 4.04 g/mol
oxygen:	3 x 16.00 g/mol	= 48.00 g/mol
nitrogen:	2 x 14.01 g/mol	= 28.02 g/mol
molecular weight		= 80.08 g/mol

How much does 2.5 mol NH_4NO_3 weigh?

(2.5 mol) x (80.08 g/mol) = 200.2 g

Mole-Mass Conversions

What is the mass of 23.706 mol C_2H_6?

$$23.706\ \cancel{\text{mol}}\ C_2H_6 \ \frac{(30.069\ \text{g})}{(1\ \cancel{\text{mol}}\ C_2H_6)}$$

$$= 712.82\ \text{g}\ C_2H_6$$

- mass ⇒ moles: divide by molar mass
- moles ⇒ mass: multiply by molar mass

Energetics of Chemical Reactions

- When a chemical reaction occurs, energy may be either absorbed by the process or released as heat into the surroundings
- The amount of energy released or absorbed depends on which chemical bonds are broken and formed
- The bond energy of a chemical bond is the amount of energy required to break that particular bond.

Energetics of Chemical Reactions

Average bond energy (kJ mol^{-1})

	single bond	double bond	triple bond
C-H	414		
C-C	347	598	837
C-O	336	803	1073
C-N	285	616	866
N-N	159	418	946
N-O	201	631	
C-S	272	575	

More are listed in Table 9.1 (p. 285)

Energetics of Chemical Reactions

Example:

$F + H_2 \rightarrow HF + H$

- In this simple reaction, we must break a H-H bond on the reactant side of the chemical equation, and form a H-F bond on the product side of the chemical equation
- We can use bond energies to calculate the net energy of this reaction

E(H-H bond) = 436 kJ/mol

E(H-F bond) = 569 kJ/mol

Energetics of Chemical Reactions

Example:

$F + H_2 \rightarrow HF + H$

E(H-H bond) = 436 kJ/mol

E(H-F bond) = 569 kJ/mol

- In order to break the H-H bond, we must put 436 kJ/mol of energy into the molecule
  - When energy is put into the system, the energy is given a positive value by convention
- When the H-F bond is formed, we get 569 kJ/mol of energy out of the system
  - When energy is released by the system, the energy is given a negative value

Energetics of Chemical Reactions

Example:

$F + H_2 \rightarrow HF + H$

E(H-H bond) = 436 kJ/mol

E(H-F bond) = 569 kJ/mol

- We can now calculate the net energy of the reaction:

  E_{rxn} = +436 kJ/mol – 569 kJ/mol = -133 kJ/mol
- Because the net energy of the reaction is negative, the energy is released to the surroundings
- In this reaction, 133 kJ/mol of energy, in the form of heat, is released to the surroundings

Energetics of Chemical Reactions

Example:

$F + H_2 \rightarrow HF + H$

- We call the heat released or absorbed by a chemical reaction the ***enthalpy of reaction*** and give it the symbol ΔH_{rxn}
- For this reaction, we would write:

  $F + H_2 \rightarrow HF + H$ $\quad\quad$ ΔH_{rxn} = -133 kJ/mol

Energetics of Chemical Reactions

Example:

$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$

Bonds broken	Bond Energy	Total Energy
4 C-H	414 kJ/mol	1656 kJ/mol
2 O=O	498 kJ/mol	996 kJ/mol
	total energy	2652 kJ/mol
Bonds formed		
2 C=O	-803 kJ/mol	-1606 kJ/mol
4 O-H	-464 kJ/mol	-1856 kJ/mol
	total energy	-3462 kJ/mol

Energetics of Chemical Reactions

Example:

$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$

ΔH_{rxn} = 2652 kJ/mol – 3462 kJ/mol = -810 kJ/mol

- Note that the enthalpy of reaction is negative, so the chemical reaction gives off heat

Energetics of Chemical Reactions

Example:

$CO_2 + H_2O \rightarrow H_2CO_3$

H – O – C – O – H
‖
O

Bonds broken	Bond Energy	Total Energy
2 C=O	803 kJ/mol	1606 kJ/mol
2 O-H	464 kJ/mol	928 kJ/mol
	total energy	2534 kJ/mol

Energetics of Chemical Reactions

Example:

$CO_2 + H_2O \rightarrow H_2CO_2$

H – O – C – O – H
‖
O

Bonds formed	Bond Energy	Total Energy
1 C=O	-803 kJ/mol	-803 kJ/mol
2 C-O	-336 kJ/mol	-672 kJ/mol
2 O-H	-464 kJ/mol	-928 kJ/mol
	total energy	-2403 kJ/mol

Energetics of Chemical Reactions

Example:

$CO_2 + H_2O \rightarrow H_2CO_2$ H – O – C – O – H

ll

O

ΔH_{rxn} = 2534 kJ/mol – 2403 kJ/mol = 131 kJ/mol

- Note that we must put 131 kJ/mol of heat into the reactants in order to make this reaction proceed to products

Energetics of Chemical Reactions

- Reactions for which the enthalpy of reaction is a positive number are called endothermic reactions
- Reactions for which the enthalpy of reaction is a negative number are called exothermic reactions

Endothermic rxn: $\Delta H_{rxn} > 0$

Exothermic rxn: $\Delta H_{rxn} < 0$