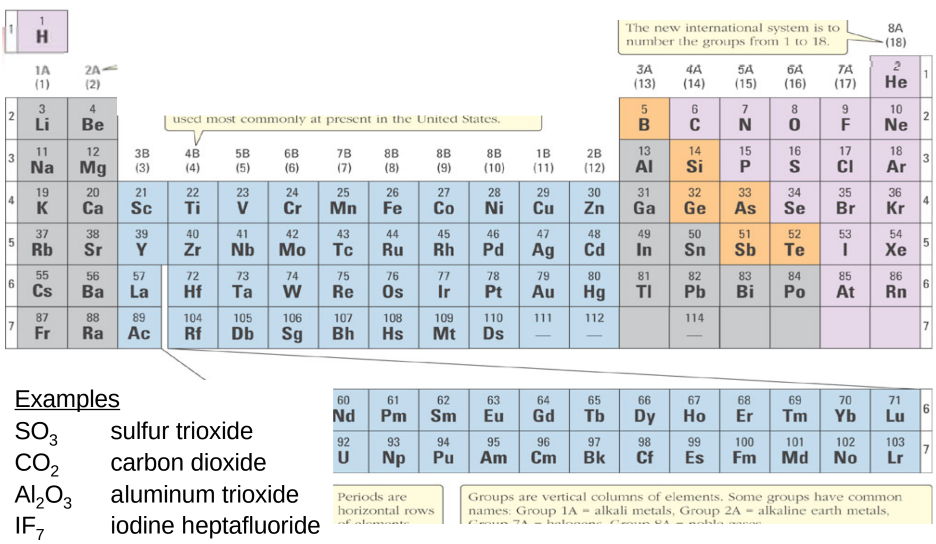
Usual Atomic Charges of Main Group Elements

+1 +2 +3 +4 +5 +6 +7

-5 -4 -3 -2 -1



<u>Examples</u>

SO_3	sulfur trioxide
CO_2	carbon dioxide
Al_2O_3	aluminum trioxide
IF_7	iodine heptafluoride

Chemical Equations

A chemical equation—just like a mathematical equation—is a way to express, in symbolic form, the reactions occurring in a chemical system.

- Balancing chemical equations
- Reaction stoichiometry
- Reagents limiting the extent of reaction
- Acid-base reactions
- Oxidation states of reactants and products

Types of Chemical Reactions

- Combination Reactions:

  Atoms or molecules combine to form a new molecule

  $2H_2 + O_2 \rightarrow 2H_2O$

  $ClO + NO_2 \rightarrow ClNO_3$

  $ClO + ClO \rightarrow ClOOCl$

Types of Chemical Reactions

- Decomposition Reactions:

  A molecule breaks apart to form different molecules or atoms

  NO_2 + sunlight $\rightarrow O + NO$

  $2C_7H_5(NO_2)_3$ + heat

  $\rightarrow 7CO(g) + 7C + 5H_2O(g) + 3N_2(g)$

Types of Chemical Reactions

- Displacement Reactions:

  An atom or molecule displaces an atom or molecule in the reaction partner

  $H + Cl_2 \rightarrow HCl + Cl$

  $2Na(s) + 2H_2O(\ell) \rightarrow 2NaOH(aq) + H_2(g)$

Types of Chemical Reactions

- Exchange Reactions:

  The components of two compounds are exchanged

  $BaCl_2(aq) + Na_2SO_4(aq)$
  $\rightarrow BaSO_4(s) + 2NaCl(aq)$

  $3NaOH(aq) + H_3PO_4(aq)$
  $\rightarrow Na_3PO_4(aq) + 3H_2O(\ell)$

Balancing Chemical Equations

- Remember *Conservation of Mass* rule—matter is neither created nor destroyed in a chemical reaction.
- A **balanced** chemical equation must have the same number of each type of atom on the reactant side as on the product side.

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

Balanced Chemical Equations

Examples

Write a balanced chemical equation for the reaction of Fe(III) with oxygen to form iron oxide

1. $Fe + O_2 \rightarrow Fe_2O_3$
2. $2\ Fe + O_2 \rightarrow Fe_2O_3$ Fe is currently balanced
3. $2\ Fe + 3/2\ O_2 \rightarrow Fe_2O_3$ O is now balanced

coefficients must usually be integer numbers—multiply everything by 2 to remove 3/2 denominator:

$4\ Fe + 3\ O_2 \rightarrow 2\ Fe_2O_3$

Balanced Chemical Equations

Examples

Write a balanced chemical equation for the combustion of methane—combustion is reaction with oxygen producing a flame. Complete combustion produces only CO_2 and H_2O.

Balanced Chemical Equations

Examples

1. $CH_4 + O_2 \rightarrow CO_2 + H_2O$

2a. $CH_4 + O_2 \rightarrow CO_2 + H_2O$ C is now balanced

2b. $CH_4 + O_2 \rightarrow CO_2 + 2\ H_2O$ H is now balanced

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

O is now balanced

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

Balanced Chemical Equations

Examples

Combustion of propane, C_3H_8

1. $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$

2a. $C_3H_8 + O_2 \rightarrow 3\ CO_2 + H_2O$

2b. $C_3H_8 + O_2 \rightarrow 3\ CO_2 + 4\ H_2O$

3. $C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$

4. No charges to balance

$C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$

Balanced Chemical Equations

Examples

Reaction of ammonium perchlorate with aluminum

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

2a. Balance N:

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

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

2b. Balance Cl:

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

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

Balanced Chemical Equations

Examples

Reaction of ammonium perchlorate with aluminum (con't.)

2c. Balance H:

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

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

2d. Balance O:

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

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

Balanced Chemical Equations

Examples

Reaction of ammonium perchlorate with aluminum (con't.)

3a. Balance Al:

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

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

3b. 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

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

1. As written, the only element out of balance is the hydrogen—balance H first:

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

2. 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)

Stoichiometry of Chemical Reactions

For the generic chemical reaction

aA + bB + … → xX + yY + …

A, B, X, and Y represent the atoms or molecules reacting and forming, and the coefficients a, b, x, and y represent the stoichiometric coefficients—they tell how many moles of one substance reacts with another substance to form some number of moles of the products.

Stoichiometry

It is important to remember that the stoichiometric coefficients represent *numbers of moles*, not masses of reactants and products

Stoichiometry

How much carbon dioxide is produced by burning one gallon of gasoline?

- Gasoline is composed of many hydrocarbons, but let's assume they are all iso-octane (C_8H_{18})
- Isooctane has a density of 0.6980 g mL^{-1}
- 1 gal = 3.785 L = 3785 mL

Stoichiometry

- Mass of isooctane

  (0.6980 g mL^{-1}) (3785 mL) = 2642 g C_8H_{18}
- Molar mass:

  8(12.011 g mol^{-1}) + 18(1.0079 g mol^{-1})

  = 114.230 g mol^{-1}
- Moles C_8H_{18}:

  (2642 g) / (114.230 g mol^{-1}) = 23.13 mol C_8H_{18}

Stoichiometry

- Balanced chemical equation:

  $2\ C_8H_{18} + 25\ O_2 \rightarrow 16\ CO_2 + 18\ H_2O$

- Determine moles of CO_2 produced:

$$(23.13\ \text{mol}\ C_8H_{18}) \frac{(16\ \text{mol}\ CO_2)}{(2\ \text{mol}\ C_8H_{18})} = 185.0\ \text{mol}\ CO_2$$

Stoichiometry

- Determine mass of CO_2:

  $(185.0\ \text{mol}\ CO_2)\ (44.009\ \text{g mol}^{-1})$

  $= 8142\ \text{g}\ CO_2 = 8.142\ \text{kg}\ CO_2$ per gallon of gasoline consumed

- How much CO_2 is emitted by CA every year?

  Californians consume ~1.4×10^{10} gallons of gasoline each year.

  $(1.4 \times 10^{10}\ \text{gal})\ (8.142\ \text{kg}\ CO_2\ \text{gal}^{-1})$

  $= 1.1 \times 10^{11}\ \text{kg}\ CO_2$

Stoichiometry

- The following general expression applies to stoichiometry problems:

$$\text{Moles B} = \frac{\text{(Coefficient B)}}{\text{(Coefficient A)}} \text{ (Moles A)}$$

Limiting Reagents

- Suppose the amount of one the reactant in a chemical reaction is insufficient to allow the reaction to proceed to completion. That reactant is called the *limiting reagent*. The limiting reagent limits how much product can formed in a reaction.

Limiting Reagents

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

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

- If we begin with 1.00 kg ammonium perchlorate and 0.100 kg aluminum, how many moles of gaseous product will be produced?

1. Which reactant will be consumed first?

   $(1000\ g\ NH_4ClO_4)/(117.488\ g\ mol^{-1}) = 8.51\ mol\ NH_4ClO_4$

   $(100\ g\ Al)/(26.982\ g\ mol^{-1}) = 3.71\ mol\ Al$

Limiting Reagents

1a. How much Al required for NH_4ClO_4 to react completely?

$$(8.51\ mol\ NH_4ClO_4)\ \frac{(10\ mol\ Al)}{(6\ mol\ NH_4ClO_4)} = 14.2\ mol\ Al$$

Since we only have 3.71 mol Al, there is insufficient Al for the NH_4ClO_4 to react completely, so Al is the limiting reagent.

2. Determine moles of each gaseous product formed in reaction:

Limiting Reagents

$$(3.71 \text{ mol Al}) \frac{(3 \text{ mol } N_2)}{(10 \text{ mol Al})} = 1.11 \text{ mol } N_2$$

$$(3.71 \text{ mol Al}) \frac{(6 \text{ mol HCl})}{(10 \text{ mol Al})} = 2.23 \text{ mol HCl}$$

$$(3.71 \text{ mol Al}) \frac{(9 \text{ mol } H_2O)}{(10 \text{ mol Al})} = 3.34 \text{ mol } H_2O$$

Total gas phase product = 6.68 mol

Limiting Reagents

Example

Ammonia reacts with nitric oxide to form nitrogen gas and water:

$NH_3 + NO \rightarrow N_2 + H_2O$

If 71.4 g NH_3 reacts with 168.6 g NO, how much N_2 and H_2O will be produced?

Step 1: Balance the chemical equation

Limiting Reagents

Example (con't.): $NH_3 + NO \rightarrow N_2 + H_2O$

Step 1: Balance the chemical equation

$2\ NH_3 + NO \rightarrow N_2 + 3\ H_2O$ H balanced

$2\ NH_3 + 3\ NO \rightarrow N_2 + 3\ H_2O$ O balanced

$2\ NH_3 + 3\ NO \rightarrow 5/2\ N_2 + 3\ H_2O$ N balanced

$4\ NH_3 + 6\ NO \rightarrow 5\ N_2 + 6\ H_2O$

remove fractional coefficient

Limiting Reagents

Example (con't.): $NH_3 + NO \rightarrow N_2 + H_2O$

Step 2: Determine moles of reactants

$$\frac{71.4 \text{ g NH}_3}{17.031\ g/mol} = 4.19 \text{ mol NH}_3 w$$

$$\frac{168.6 \text{ g NO}}{30.006 \text{ g/mol}} = 5.62 \text{ mol NO}$$

Step 3: Determine which is limiting reagent

$$(5.62 \text{ mol NO}) \frac{(4 \text{ mol NH}_3)}{(6 \text{ mol NO})} = 3.75 \text{ mol NH}_3$$

NO is limiting reagent

Limiting Reagents

Example (con't.): $NH_3 + NO \rightarrow N_2 + H_2O$

Step 4: Determine amount of products

$$(5.62 \text{ mol NO}) \frac{(5 \text{ mol } N_2)}{(6 \text{ mol NO})} = 4.68 \text{ mol } N_2$$

$$(4.68 \text{ mol } N_2)(28.014 \text{ g/mol}) = 131 \text{ g } N_2$$

$$(5.62 \text{ mol NO}) \frac{(6 \text{ mol } H_2O)}{(6 \text{ mol NO})} = 5.62 \text{ mol } H_2O$$

$$(5.62 \text{ mol } H_2O)(18.0152 \text{ g/mol}) = 101 \text{ g } H_2O$$

Limiting Reagents

Example

$Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

compound	initial mass	initial moles
$Ca_5(PO_4)_3F$	1000. g	1.983 mol
H_2SO_4	200.0 g	2.039 mol
H_2O	100.0 g	5.551 mol

Determine mass of all products formed

Limiting Reagents

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

Step 1: Determine limiting reagent—examine $Ca_5(PO_4)_3F$

$$(1.983\text{ mol Ca}_5\text{...})\ \frac{(5\text{ mol H}_2\text{SO}_4)}{(1\text{ mol Ca}_5\text{...})} = 9.915\text{ mol H}_2\text{SO}_4\text{ for complete rxn}$$

$$(1.983\text{ mol Ca}_5\text{...})\ \frac{(10\text{ mol H}_2\text{O})}{(1\text{ mol Ca}_5\text{...})} = 19.83\text{ mol H}_2\text{O for complete rxn}$$

Not enough H_2SO_4 or H_2O to react completely with $Ca_5(PO_4)_3F$
$\therefore Ca_5(PO_4)_3F$ is not limiting reagent

Limiting Reagents

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

Step 1: Determine limiting reagent—examine H_2SO_4

$$(2.039\text{ mol H}_2\text{SO}_4)\ \frac{(10\text{ mol H}_2\text{O})}{(5\text{ mol H}_2\text{SO}_4)} = 4.078\text{ mol H}_2\text{O for complete rxn}$$

H_2O is in excess relative to the amount needed to react completely with H_2SO_4
$\therefore H_2SO_4$ is limiting reagent

Limiting Reagents

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

Step 2: Determine amount of product formed

$$(2.039 \text{ mol } H_2SO_4)\ \frac{(3 \text{ mol } H_3PO_4)}{(5 \text{ mol } H_2SO_4)} = 1.223 \text{ mol } H_3PO_4 \text{ w}$$

$$(1.223 \text{ mol } H_3PO_4)\ (97.995 \text{ g/mol}) = 119.8 \text{ g } H_3PO_4$$

Limiting Reagents

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

Step 2: Determine amount of product formed

$$(2.039 \text{ mol } H_2SO_4)\ \frac{(5 \text{ mol } CaSO_4 \cdot 2H_2O)}{(5 \text{ mol } H_2SO_4)} = 2.039 \text{ mol } CaSO_4$$

$$(2.039 \text{ mol } CaSO_4 \cdot 2H_2O)\ (172.17 \text{ g/mol}) = 351.1 \text{ g } CaSO_4 \cdot 2H_2O$$

$$(2.039 \text{ mol } H_2SO_4)\ \frac{(1 \text{ mol HF})}{(5 \text{ mol } H_2SO_4)} = 0.4078 \text{ mol HF}$$

$$(0.4078 \text{ mol HF})\ (20.006 \text{ g/mol}) = 8.158 \text{ g HF}$$

Product Yields

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

For each kg of $Ca_5(PO_4)_3F$ that reacts, 400. g of phosphoric acid are formed. What is the percent yield of phosphoric acid?

Product Yields

Example: $Ca_5(PO_4)_3F + 5\ H_2SO_4 + 10\ H_2O$

$\rightarrow 3\ H_3PO_4 + 5\ CaSO_4{\cdot}2H_2O + HF$

Step 1: Determine the theoretical yield—amount of product formed if reaction occurred completely

$$(1.983 \text{ mol } Ca_5...) \frac{(3 \text{ mol } H_3PO_4)}{(1 \text{ mol } Ca_5...)} = 5.949 \text{ mol } H_3PO_4 \text{ for complete rxn}$$

$$(5.949 \text{ mol } H_3PO_4)\ (97.995 \text{ g/mol}) = 583 \text{ g } H_3PO_4 \text{ theoretical yield}$$

$$\%\ \text{yield} = \frac{\text{actual yield}}{\text{theory yield}} \times 100\% = \frac{400\text{ g}}{583\text{ g}} \times 100\% = 68.6\%$$