Chemistry Lecture #85: Calculation of Reaction Rate & the Rate Law

Reaction rate is the rate at which product is made in a chemical reaction. It can also be the rate at which reactant is consumed.

If we know the change in the concentration of product and the time it takes for the amount to change, the average reaction rate can be calculated using

$$\text{Average reaction rate} = \frac{\Delta\text{quantity}}{\Delta t}$$

Δquantity = change in concentration of product or reactant. Units are expressed in moles/liter, which is represented by [ ]. Change in quantity is expressed as a positive number.

Δt = change in time, or time needed for the amount of product/reactant to change. Time is measured in seconds.

The reaction

$H_2 + Cl_2 \rightarrow 2HCl$

takes place in a container. The chart below shows the concentrations of H_2, Cl_2, HCl at t = 0 seconds and t = 4 seconds.

Time	$[H_2]$	$[Cl_2]$	$[HCl]$
0.00 s	0.030 M	0.050 M	0.00 M
4.00 s	0.020 M	0.040 M	0.020 M

(a) Calculate the average reaction rate expressed in moles H_2 consumed per liter per second.

(b) Calculate the average reaction rate expressed in moles HCl produced per liter per second.

Answer

For part (a),

$$\text{Average reaction rate} = \frac{\Delta \text{quantity}}{\Delta t} = \frac{0.020 - 0.030}{4.00 - 0.00}$$

$$= -0.0025 \text{ or } +0.0025 \text{ mol/(L s)}$$

For part (b),

$$\text{Average reaction rate} = \frac{\Delta \text{quantity}}{\Delta t} = \frac{0.020 - 0.000}{4.00 - 0.00}$$

$$= 0.0050 \text{ mol/(L s)}$$

Thus, H_2 disappears at a rate of 0.0025 mol/(L s), and HCl appears at a rate of 0.0050 mol/(L s).

A high concentration of reactants will make a reaction go faster. As the reactants get used up, the reaction proceeds more slowly. The rate of a chemical reaction at a particular concentration of reactants can be calculated using the rate law for a reaction. Suppose we have a chemical reaction where

$A + B \rightarrow C$

The rate law for the reaction would be

$\text{Rate} = k[A]^x [B]^y$

Rate = Instantaneous rate at which the concentration of reactant disappears (or product appears) at a particular concentration of reactants.

k = specific rate constant. This is a number that relates reaction rate and concentration of reactants at a given temperature.

[A] = concentration of reactant A
x = order of the reaction for reactant A
[B] = concentration of reactant B
y = order of the reaction for reactant B

The values of x and y are usually 0, 1, or 2. Sometimes the numbers are fractions or negative numbers. These numbers are referred to as "orders." If x = 1, then reactant A is first order. If y = 2, then reactant B is 2nd order. The overall order would be x + y or 1 + 2 = 3.

The rate law for the reaction

$$2NO\ (g) + H_2(g) \rightarrow N_2O\ (g) + H_2O\ (g)$$

is rate = $k[NO]^2\ [H_2]$, where $k = 2.90 \times 10^2\ (L^2/(mol^2\ s))$. Find the instantaneous rate of reaction when $[NO] = 0.00200$ M and $[H_2] = 0.00400$ M.

Answer

$$\text{rate} = k[NO]^2\ [H_2]$$

$$\text{rate} = 2.90 \times 10^2\ (L^2/(mol^2\ s))\ (0.00200\ mol/L)^2\ (0.00400\ mol/L)$$

$$\text{rate} = (2.90 \times 10^2)\ (0.00200)^2\ (0.00400)$$

$$\text{rate} = 4.64 \times 10^{-6}\ mol/(L\ s)$$

This is the reaction rate at the exact moment when $[NO] = 0.00200$ M and $[H_2] = 0.00400$ M. A split second later, the reaction rate will slow down since NO and H_2 are consumed in the reaction, causing their concentration to decrease.

The rate law for a reaction is determined experimentally. Reaction rates are measured at one concentration, then run again with the concentration of reactants doubled.

If doubling the concentration of a reactant has no effect on the rate, the order of the reactant is zero. Doubling the concentration is equivalent to multiplying the rate by 1. $2^0 = 1$.

If doubling the concentration of a reactant doubles the rate, the order of the reactant is one. Doubling the concentration is equivalent to multiplying the rate by 2. $2^1 = 2$.

If doubling the concentration of a reactant quadruples the rate, the order of the reactant is two. Doubling the concentration is equivalent to multiplying the rate by 4. $2^2 = 4$.

Use the data table below to find the rate law for the reaction

$CH_3COCH_3 + I_2 \rightarrow CH_3COCH_2I + HI$

Trial	$[CH_3COCH_3]$ M	$[I_2]$ M	Rate mol/(L s)
1	0.0500	0.0500	5.78×10^{-8}
2	0.0500	0.100	5.78×10^{-8}
3	0.100	0.1 00	1.16×10^{-7}

Compare trials 1 and 2. Between the trials, the concentration of I_2 is doubled from 0.0500 M to 0.100 M while the concentration of CH_3COCH_3 is kept constant at 0.0500 M. The reaction rate stayed the same at 5.78×10^{-8} mol/(L s) - it was as though the rate had been multiplied by 1 or 2^0. Since doubling the concentration of I_2 had no effect on the reaction rate, the order for I_2 is zero. We record the result as $[I_2]^0$.

Compare trials 2 and 3. Between the trials, the concentration of CH_3COCH_3 is doubled from 0.0500 M to 0.100 M while the concentration of I_2 is kept constant at 0.100 M. The reaction rate increase from 5.78×10^{-8} mol/(L s) to 1.16×10^{-7} mol/(L s). $(1.16 \times 10^{-7})/(5.78 \times 10^{-8}) = 2$ or 2^1. Since doubling the concentration of CH_3COCH_3 doubled the reaction rate, the order for CH_3COCH_3 one. We record the result as $[CH_3COCH_3]^1$, or just $[CH_3COCH_3]$.

The rate law is thus

Rate = $k[CH_3COCH_3][I_2]^0$. Since $[I_2]^0 = 1$, we write

Rate = $k[CH_3COCH_3]$

Use the data table below to find the rate law and the specific rate constant for the reaction

$2NO + Cl_2 \rightarrow 2NOCl$

Trial	[NO] M	[Cl_2] M	rate mol/(L s)
1	0.50	0.50	0.0190
2	1.00	0.50	0.0760
3	1.00	1.00	0.1520

From trial 1 to 2, [NO] is doubled from 0.50 M to 1.00 M. The rate is 4 times faster (0.0760/0.0190 = 4 or 2^2). The order for NO is 2, so we write $[NO]^2$.

From trial 2 to 3, [Cl_2] is doubled from 0.50 M to 1.00 M. The rate is 2 times faster (0.1520/0.0760 = 2 or 2^1). The order for [Cl_2] is 1, so we write $[Cl_2]^1$ or just [Cl_2].

The rate law is Rate = $k[NO]^2\,[Cl_2]$.

The value of k can be found by substituting the concentrations and rate from any trial. We'll use the data from trial 1.

$$\text{Rate} = k[NO]^2\,[Cl_2]$$

$$0.0190 = k[0.50]^2\,[0.50]$$

$$k = \frac{0.0190}{[0.50]^2\,[0.50]} = 0.152\ L^2/(mol^2\ s)$$