CHEMICAL KINETICS

THE RATES AND MECHANISMS OF CHEMICAL REACTIONS

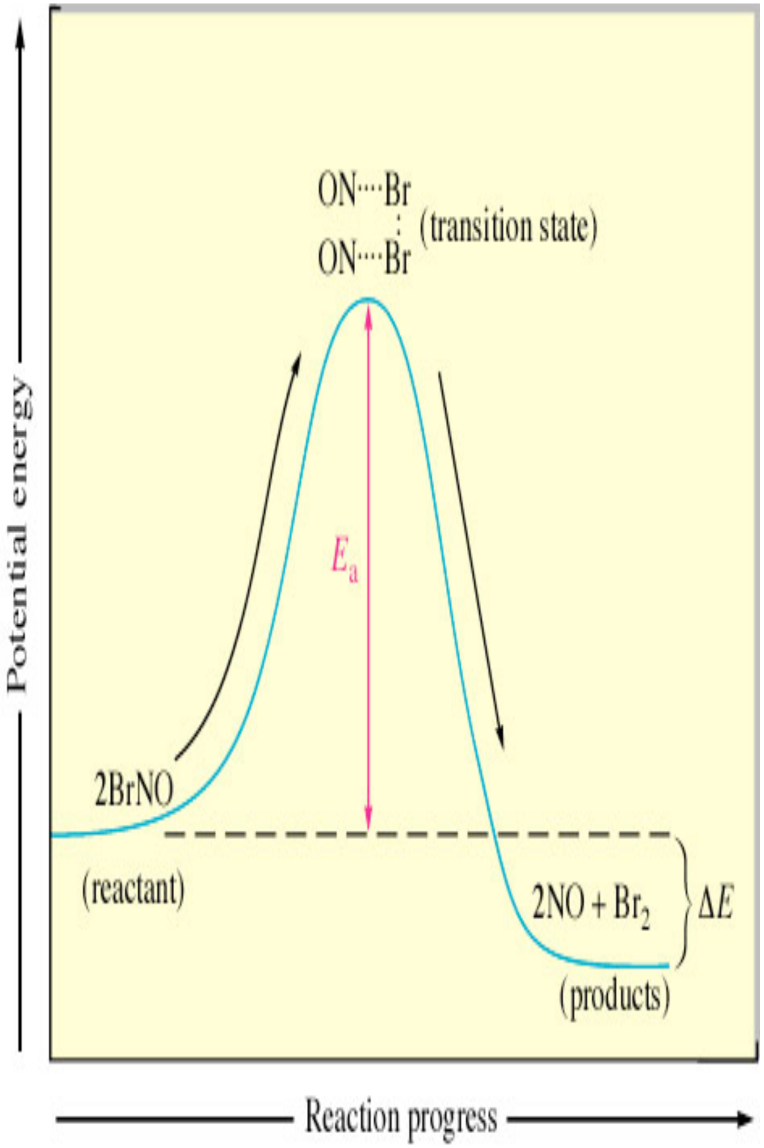
Chemical kinetics is the study of the speed or rate of a reaction under various conditions.

THE COLLISION THEORY OF REACTION RATES

- Particles must collide.
- Only two particles may collide at one time.
- Proper orientation of colliding molecules so that atoms can come in contact with each other to become products.

The collision must occur with enough energy to overcome the electron/electron repulsion of the valence shell electrons of the reacting species and must have enough energy to transform translational energy into vibrational energy in order to penetrate into each other so that the electrons can rearrange and form new bonds.

This new collision product is at the peak of the activation energy hump and is called the *activated complex* or the transition state. At this point, the *activated complex* can still either fall to reactants or to products.



REACTION MECHANISMS

The sequence of bond-making and bond-breaking steps that occurs during the conversion of reactants to products.

Must be determined by experiment!

Must agree with overall stoichiometry AND the experimentally determined rate law!

ELEMENTARY STEPS

Molecularity--number of molecules that participate in an atomic rearrangement

- unimolecular: involves one reactant molecule
- bimolecular: involves a collision between two reactant molecules
- termolecular: simultaneous collision between three reactant molecules **[very rare!]***

A mechanism is a sequence of events at the molecular level that controls the speed and outcome of the reaction.

FACTORS THAT AFFECT REACTION RATES

The following conditions affect the speed of a chemical process:

1. Nature of the reactants

Some reactant molecules react in a hurry, others react very slowly.

Pointers…

Physical state -

gasoline $_{\mathbf{(l)}}$ vs. gasoline $_{\mathbf{(g)}}$

$K_2SO_{4(s)} + Ba(NO_3)_{2(s)} \rightarrow$ no rxn.

while both of these in the **aqueous state do react.

Chemical identity
What is reacting?

Usually, ions of opposite charge react very rapidly.

Usually, the more bonds between reacting atoms in a molecule, the slower the reaction rate.

Substances with strong bonds (larger bond energies) will react much more slowly.

Examples:

Metallic sodium reacts much faster with water than metallic calcium.

Oxidation of methane can be increased with an increase in temperature.

Photosynthesis is very slow and changes very little with an increase in temperature.

2. Concentration of reactants

More molecules,

More collisions.

3. Temperature

heat >em up & speed >em up

The faster they move, the more likely they are to collide.

An increase in temperature produces more successful collisions that are able to overcome the needed activation energy,

therefore,

a general increase in reaction rate with increasing temperature.

4. Catalysts

accelerate chemical reactions but are not themselves transformed.

Biological catalysts are proteins called enzymes.

A catalyst is a substance that changes the rate of reaction by altering the reaction pathway.

Most catalysts work by lowering the activation energy needed for the reaction to proceed; therefore, more collisions are successful and the reaction rate is increased.

Remember!

The catalyst is not part of the chemical reaction and is not used up during the reaction.

* (May be homogeneous or heterogeneous catalysts.)

Example…

H_2O_2 decomposes relatively slowly into
H_2O and O_2

however…

exposure to light accelerates this
process AND with the help of MnO_2, it goes extremely FAST!!

Note:

A catalyst lowers the activation energy barrier. Therefore, the forward and reverse reactions are both accelerated to the same degree.

* (Some homogeneous catalysts actually appear in the rate law because their concentration affects the reaction. Ex. NO catalyzing O_3)

5. Surface area of reactants

exposed surfaces affect speed.

Except for substances in the gaseous state or solution, reactions occur at the boundary, or interface, between two phases.

The greater surface area exposed, the greater chance of collisions between particles, hence, the reaction should proceed at a much faster rate.

Ex. coal dust is very explosive as opposed to a piece of charcoal.

Solutions are ultimate exposure!

With all of these criteria met, the reaction may proceed in the forward direction.

Amazing that we have reactions occurring at all!

RATE EXPRESSIONS FOR ELEMENTARY STEPS

The rate expression cannot be predicted from overall stoichiometry.

The rate expression of an elementary step is given by the product of the rate constant and the concentrations of the reactants in the step.

ELEMENTARY STEP	MOLECULARITY	RATE EXPRESSION
$A \rightarrow$ products	unimolecular	rate = $k[A]$
$A + B \rightarrow$ products	bimolecular	rate = $k[A][B]$
$A + A \rightarrow$ products	bimolecular	rate = $k[A]^2$
$2\,A + B \rightarrow$ products*	termolecular*	rate = $k[A]^2[B]$

MOLECULARITY AND ORDER

an **elementary step** is a reaction whose rate law can be written from its molecularity

NOT true of the overall reaction order!

Exercise

Nitrogen oxide is reduced by hydrogen to give water and nitrogen,

$$2\ H_{2(g)} + 2\ NO_{(g)} \rightarrow N_{2(g)} + 2\ H_2O_{(g)}$$

One possible mechanism to account for this reaction is:

$$2\ NO_{(g)} \leftrightarrow N_2O_{2(g)}$$

$$N_2O_{2(g)} + H_{2(g)} \rightarrow N_2O_{(g)} + H_2O_{(g)}$$

$$N_2O_{(g)} + H_{2(g)} \rightarrow N_{2(g)} + H_2O_{(g)}$$

What is the molecularity of each of the three steps?

Show that the sum of these elementary steps is the net reaction.

REACTION MECHANISMS AND RATE EXPRESSIONS

- determined by experiment
- the rate of the overall reaction is limited by, and is exactly equal to, the combined rates of all elementary steps ***up to and including the slowest step in the mechanism***

- the slowest step is the **rate determining step**
- **reaction intermediate**--produced in one step but consumed in another.
- **catalyst**--goes in, comes out unharmed and DOES NOT show up in the final rxn.

Exercise

The balanced equation for the reaction of the gases nitrogen dioxide and fluorine is

$$2\ NO_2\ (g)\ +\ F_2\ (g)\ \rightarrow\ 2\ NO_2F\ (g)$$

The *experimentally* determined rate law is

$$\text{Rate} = k\ [NO_2][F_2]$$

Exercise Continued

A suggested mechanism for the reaction is

$NO_2 + F_2 \rightarrow NO_2F + F$ Slow

$F + NO_2 \rightarrow NO_2F$ Fast

Is this an acceptable mechanism? That is, does it satisfy the two requirements?

Justify.

CHEMICAL REACTION RATES

The speed of a reaction is expressed in terms of its “rate”, some measurable quantity is changing with time.

The rate of a chemical reaction is measured by the decrease in concentration of a reactant or an increase in concentration of a product in a unit of time.

Rate =

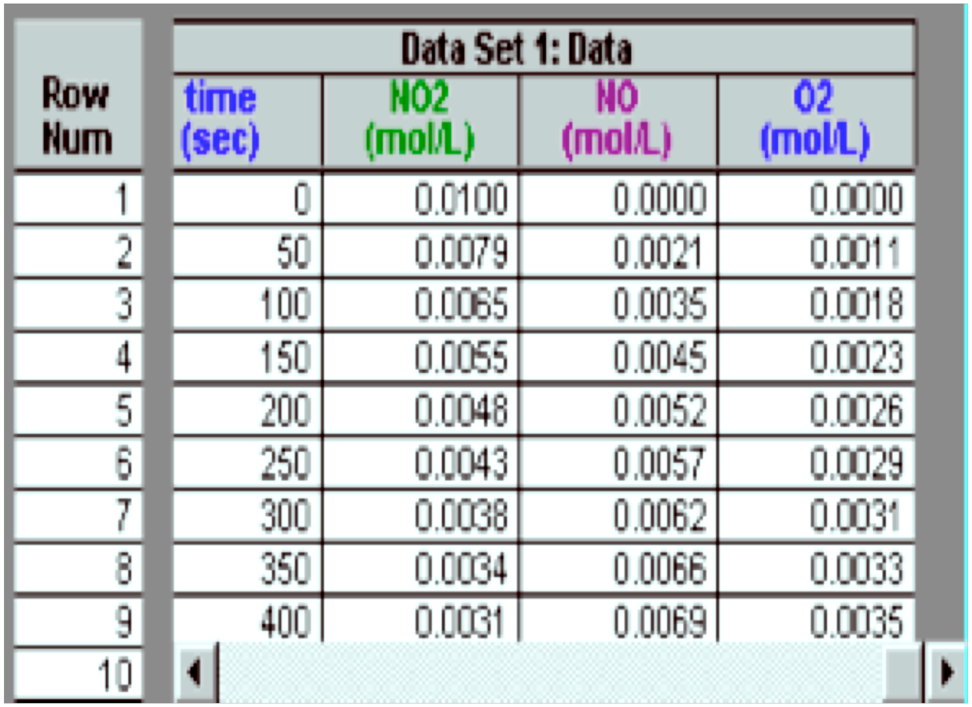
$$\text{Rate} = \frac{\text{change in concentration of a species}}{\text{time interval}}$$

When writing rate expressions, they can be written in terms of reactants disappearance or products appearance.

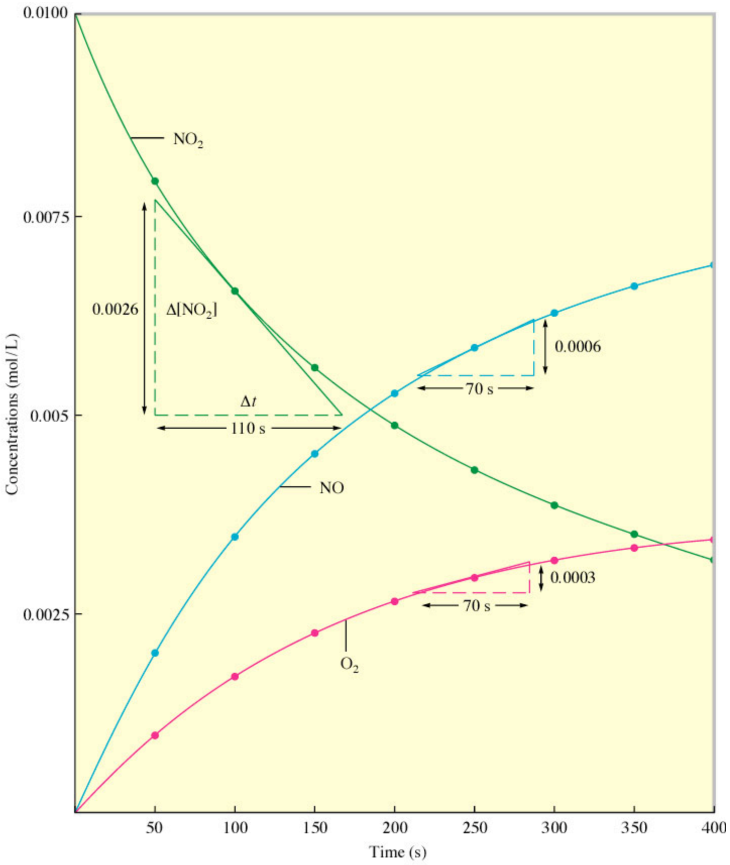
Rate is not constant, it changes with time. Graphing the data of an experiment will show an average rate of reaction.

You can find the instantaneous rate by computing the slope of a straight line tangent to the curve at that time.

Graph of Experimental Data



Row Num	Data Set 1: Data			
	time (sec)	NO2 (mol/L)	NO (mol/L)	O2 (mol/L)
1	0	0.0100	0.0000	0.0000
2	50	0.0079	0.0021	0.0011
3	100	0.0065	0.0035	0.0018
4	150	0.0055	0.0045	0.0023
5	200	0.0048	0.0052	0.0026
6	250	0.0043	0.0057	0.0029
7	300	0.0038	0.0062	0.0031
8	350	0.0034	0.0066	0.0033
9	400	0.0031	0.0069	0.0035
10				



Reaction Rate

Expressed as the Δ in concentration of a reagent per unit time or Δ[A]/Δt

Focus either on the disappearance of reactants or the appearance of products

- rate of Δ of a reactant is always *negative*
- rate of Δ of a product is always *positive*

Consider:

$$2\ NO_{2(g)} \rightarrow O_{2(g)} + 2\ NO_{(g)}$$

- Oxygen can appear only half as rapidly as the nitrogen dioxide disappears
- NO appears twice as fast as oxygen appears.

Calculate the **AVERAGE** rate at which $[NO_2]$ changes in the first 50.0 seconds:

$$\text{RATE} = \frac{\Delta\,[NO_2]}{\Delta t} = \frac{[.0079]-[0.0100]}{50.0\ \text{s}}$$

$$= -[-4.2 \times 10^{-5}\ \text{mol/L} \bullet \text{sec}]$$

$$= 4.2 \times 10^{-5}\ \text{mol/L} \bullet \text{sec}$$

or, M • s-1

Note that the rate is *NOT* constant but decreases with time.

The rates given below are *average* rates.

$-\frac{\_[NO_2]}{\_t}$ (x 10^{-5})	Time period (s)
4.2	0 _ 50
2.8	50 _ 100
2.0	100 _ 150
1.4	150 _ 200

To find the value of the rate at a particular time, the **instantaneous rate**, compute the slope of a line tangent to the curve at that point.

Why the negative on NO_2?

RELATIVE RATES

We can consider the appearance of products along with the disappearance of reactants.

The reactant’s concentration is declining, the product’s is increasing.

Respect the algebraic sign AND respect the stoichiometry.

Divide the rate of change in concentration of each reactant by its stoichiometric coefficient in the balanced chem. eqn. and this is foolproof and a breeze!

Thus...

Rate of Reaction =

$$- \frac{1\Delta[NO_2]}{2\ \Delta time} = \frac{1\ \Delta[NO]}{2\ \Delta time} = \frac{\Delta[O2]}{\Delta time}$$

Of course you can change these once the ratio is set. You might prefer:

$$-1 : +1 : +2$$

Relative Rates from the balanced equation:

Using the coefficients from the balanced equation, you should be able to give relative rates.

For example:

$$4\ PH_{3\,(g)} \rightarrow P_{4(g)} + 6\ H_{2(g)}$$

Initial rate rxn. =

$$\text{Initial rate rxn.} = -\frac{1}{4}\left[\frac{\Delta[PH_3]}{\Delta time}\right] = +\left[\frac{[P_4]}{\Delta time}\right] = +\frac{1}{6}\left[\frac{\Delta[H_2]}{\Delta time}\right]$$

Exercise

What are the *relative* rates of change in concentration of the products and reactant in the decomposition of Nitrosyl chloride, NOCl?

$$2\ NOCl_{(g)} \rightarrow 2\ NO_{(g)} + Cl_{2(g)}$$

Initial Reaction Rates

Begin with pure reactants, mix thoroughly, then measure speed of rxn. Over time, the presence of products can alter results dramatically and lead to confusing results.

We'll be talking initial reaction rates throughout our discussions!

Rate expression or rate law is the relation between reaction rate and the concentrations of reactants given by a mathematical equation.

CONCENTRATION AND REACTION RATE:

THE RATE LAW OR RATE EXPRESSION:

Rates generally depend on reactant concentrations.

To find the exact relation between rate and concentration, we must **do some experiments** and collect information.

Initial rxn rate = $k[A]^m[B]^n[C]^p$

k = rate constant

[A] = concentration of reactant A

[B] = concentration of reactant B

[C] = concentration of the catalyst—won’t see this too often

m = order of reaction for reactant A

n = order of reaction for reactant B

p = order of reaction for the catalyst C

Exponents can be zero, whole numbers, or fractions --

AND MUST BE DETERMINED BY EXPERIMENTATION!!

THE RATE CONSTANT, *k*

Is temperature dependent & must be evaluated by experiment.

Example: rate = $k[Pt(NH_3)_2Cl_2]$

k = 0.090/hr, therefore when [ion] = 0.018 mol/L

rate =

(.0090/hr)(0.018 mol/L) = 0.0016 mol/(L• hr)

ORDER OF A REACTION

Order with respect to a certain reactant is the *exponent* on its concentration term in the rate expression.

Order of the reaction is the sum of all the exponents on all the concentration terms in the expression.

DETERMINATION OF THE RATE EXPRESSION

$$aA + bB \rightarrow xX$$

$$\text{initial rate} = k[A]_o^m[B]_o^n$$

the little subscript “o” means original.

Zero order

- The change in concentration of reactant has no effect on the rate.
- These are not very common.
- General form of rate equation:

$$\textbf{Rate} = \mathbf{k}$$

First order

- Rate is directly proportional to the reactants concentration; doubling [rxt], doubles rate. These are very common! Nuclear decay reactions usually fit into this category.

- General form of rate equation:

$$\textbf{Rate} = \mathbf{k}\ [\mathbf{A}]$$

Second order

- Rate is quadrupled when [rxt] is doubled and increases by a factor of 9 when [rxt] is tripled, etc. These are common, particularly in gas-phase reactions.
- General form of rate equation:

$$\textbf{Rate} = \mathbf{k}\,[\mathbf{A}]^2$$

Fractional orders are rare!

Ex. rate = $k[A]_o^m[B]_o^n$

If m = 0 ; reaction is **zero order** with respect to A

If m = 1 ; reaction is **1st order** with respect to A

If m = 2 ; reaction is **2nd order** with respect to A

If n = 0 ; reaction is **zero order** with respect to B

If n = 1 ; reaction is **1st order** with respect to B

If n = 2 ; reaction is **2nd order** with respect to B

TWO TYPES OF RATE LAW

- **differential rate law**--expresses how the rate depends on **concentration** (most common)

- **integrated rate law**--expresses how the concentrations depend on **time**

INTEGRATED RATE LAW -

CONCENTRATION/TIME RELATIONSHIPS

When we wish to know how long a reaction must proceed to reach a predetermined concentration of some reagent, we can construct curves or derive an equation that relates concentration and time.

GRAPHICAL METHODS FOR DISTINGUISHING FIRST AND SECOND ORDER REACTIONS

First order:

$$\ln[A] = -kt + \ln[A]_o$$

$$y = ax + b$$

Second order:

$$1/[A] = kt + 1/[A]_o$$

$$y = ax + b$$

ln[reactant] vs. time produces a straight line for **first order** in that reactant &

since a = -k

the slope of the line is *negative*.

1/[reactant] vs. time produces a straight line for **second order** in that reactant &

since a = k

the slope is *positive*.

Using the graphing calculator or a graphing program such as Logger Pro

Set up your calculator so that

time is always in the first list (L1 or X) and the y-list is alphabetical!

L1 = time (x variable throughout!)

L2 = concentration: [A]

straight line = zero order

L3 = ln concentration: ln [A]

straight line = first order

L4 = reciprocal concentration: 1/[A]

straight line = second order

Run 3 linear regressions – one each for:

L1, L2

L1, L3

L1, L4

and see which has the best “r” [linear regression correlation coefficient in big people language!]

Exercise

The decomposition of N_2O_5 in the gas phase was studied at constant temperature.

$$2\ N_2O_5\ (g) \rightarrow 4\ NO_2\ (g) + O_2\ (g)$$

The following results were collected:

$[N_2O_5]$	Time (s)
0.1000	0
0.0707	50
0.0500	100
0.0250	200
0.0125	300
0.00625	400

Determine the rate law and calculate the value of *k*.

Exercise

Using the data given for the previous problem (shown below), calculate $[N_2O_5]$ at 150 s after the start of the reaction.

$[N_2O_5]$	Time (s)
0.1000	0
0.0707	50
0.0500	100
0.0250	200
0.0125	300
0.00625	400

Calculate the $[N_2O_5]$ at the following times:

200 s 400 s 600 s 1,000 s

HALF-LIFE AND REACTION RATE FOR FIRST ORDER REACTIONS, $t_{1/2}$

The time required for one half of one of the reactants to disappear.

$$[A] = \tfrac{1}{2}[A]_o \qquad \text{or} \qquad \frac{[A]}{[A]_o} = \tfrac{1}{2}$$

so... $$\ln \frac{[A]}{[A]_o/2} = k\,t_{\frac{1}{2}}$$

and... $\ln 2 = t_{\frac{1}{2}}$

Rearrange, evaluate ln 2 and solve for $t_{1/2}$ and you get

$$t_{1/2} = \frac{0.693}{k}$$

“Half life is INDEPENDENT OF **ORIGINAL C**ONCENTRATION for 1st order!!!”

Exercise

A certain first-order reaction has a half-life of 20.0 minutes.

a. Calculate the rate constant for this reaction.
b. How much time is required for this reaction to be 75% complete?

Exercise

The rate constant for the first order transformation of cyclopropane to propene is 5.40×10^{-2}/hr.

-What is the half-life of this reaction?

-What fraction of the cyclopropane remains after 51.2 hours?

-What fraction remains after 18.0 hours?

Exercise

For the reaction of $(CH_3)_3CBr$ with OH^-,

$(CH_3)_3CBr + OH^- \rightarrow (CH_3)_3COH + Br^-$

The following data were obtained in the laboratory:

TIME (s)	$[(CH_3)_3CBr]$
0	0.100
30	0.074
60	0.055
90	0.041

Plot these data as ln $[(CH_3)_3CBr]$ versus time. Sketch your graph.

Is the reaction first order or second order?

What is the value of the rate constant?

HALF-LIFE AND REACTION RATE FOR SECOND ORDER REACTIONS, t1/2

The time required for one half of one of the reactants to disappear.

$[A] = \frac{1}{2}[A]_o$ or $\frac{[A]}{[A]_o} = \frac{1}{2}$

so...

$$\frac{1}{[A]_o/2} = k\, t_{1/2} + \frac{1}{[A]_o}$$

Rearrange ,

$$\frac{2}{[A]_o} - \frac{1}{[A]_o} = k\, t_{1/2}$$

$$k\, t_{1/2} = \frac{1}{[A]_o}$$ solve for $t_{1/2}$,

$$t_{1/2} = \frac{1}{k[A]_o}$$ for a 2nd order rxn.

Exercise

Butadiene reacts to form its dimer according to the equation:

$$2\ C_4H_6\ (g) \rightarrow C_8H_{12}\ (g)$$

The following data were collected for this reaction at a given temperature:

$[C_4H_6]$	Time (± 1 s)
0.01000	0
0.00625	1000
0.00476	1800
0.00370	2800
0.00313	3600
0.00270	4400
0.00241	5200
0.00208	6200

What is the order of this reaction? Explain. Sketch your graph as part of your explanation. Write the rate law expression:

Continued:

$[C_4H_6]$	Time (± 1 s)
0.01000	0
0.00625	1000
0.00476	1800
0.00370	2800
0.00313	3600
0.00270	4400
0.00241	5200
0.00208	6200

-What is the value of the rate constant for this reaction?

-What is the half-life for the reaction under the conditions of this experiment?

INTEGRATED RATE LAWS FOR REACTIONS WITH MORE THAN ONE REACTANT

Must [still] be determined by experiment! But we use a technique called “swamping”.

This is also referred to as the “**isolation method**”.

Flood the reaction vessel with high concentrations of all but one reactant and perform the experiment.

The reactants at high concentrations like say, 1.0 M compared to the reactant with a low concentration say, 1.0 x 10^{-3} M, stay the same.

"In English"—the rate is now dependent on the concentration of the little guy since the big guy's aren't changing, therefore:

rate = *k*' [little guy]

We now re-write the rate as a **pseudo-rate-law** and *k*' is a **pseudo-rate-constant**

DIFFERENTIAL RATE LAW

- Method of Initial Rates: We measure the rate at the very beginning for different concentrations.

Experiment Number	Initial Rate mol/(L_hr)	Initial concentration $[A]_0$	Initial concentration $[B]_0$
1	0.50 x 10^{-2}	0.50	0.20
2	0.50 x 10^{-2}	0.75	0.20
3	0.50 x 10^{-2}	1.00	0.20
4	1.00 x 10^{-2}	0.50	0.40
5	1.50 x 10^{-2}	0.50	0.60

Since the rate stays the same regardless of the concentration of [A], it is zero order with respect to A.

However, the rate doubles with a doubling of [B] and triples with a tripling of [B].

This indicates the rate is first order with respect to [B].

Summary

Initial reaction rate =

$$k[A]_o^o[B]_o1 = k[B]_o^1$$

The overall reaction rate =

1 + 0 = 1st order overall.

Now. . . . .

Use a set of the data to calculate k:

$0.0050\ \text{mol/(L•hr)} = k[0.20\ \text{mol/L}]^1$

$k = 2.5 \times 10^{-2}$ /hr

You should get the same value with any set of data!

Ugly algebraic method is sometimes necessary

$$\frac{\text{rate 1}}{\text{rate 2}} = \frac{k\,[\text{reactant}]^m\,[\text{reactant}]^n}{k\,[\text{reactant}]^m\,[\text{reactant}]^n}$$

Select a trial where one reactant concentration is held constant

SO THAT IT CANCELS;

the *k*'s will also cancel.

Using trials 1 & 4:

$$\frac{0.50 \times 10^{-2}}{1.00 \times 10^{-2}} = \frac{k\,[0.50]^m\,[0.20]^n}{k\,[0.50]^m\,[0.40]^n}$$

so.... $\frac{1}{2} = [\,\frac{1}{2}\,]^n$

and ∴ n must be ONE to make that true!

Exercise

In the following reaction, a Co-Cl bond is replaced by a Co-OH_2 bond.

$$[Co(NH_3)_5Cl]^{+2} + H_2O \rightarrow$$
$$[Co(NH_3)_5H_2O]^{+3} + Cl$$

Initial rate = k $\{[Co(NH_3)_5Cl]^{+2}\}^m$

Using the data below, find the value of *m* in the rate expression and calculate the value of *k*.

Exp.	Initial Concentration of $[Co(NH_3)_5Cl]^{+2}$ (mol/L)	Initial rate mol/(L•min)
1	1.0×10^{-3}	1.3×10^{-7}
2	2.0×10^{-3}	2.6×10^{-7}
3	3.0×10^{-3}	3.9×10^{-7}
4	1.0×10^{-3}	1.3×10^{-7}

Exercise

The reaction between bromate ions and bromide ions in acidic aqueous Solution is given by the equation:

$$BrO_3^-\,(aq) + 5\,Br^-\,(aq) + 6\,H^+\,(aq) \rightarrow$$
$$3\,Br_2\,(l) + 3\,H_2O\,(l)$$

The table below gives the results of four *experiments*. Using these data, determine the orders for all three reactants, the overall reaction order, and the value of the rate constant.

What is the value of *k*? What are the units of *k*?

Experiment	Initial $[BrO_3^-]$	Initial $[Br^-]$	Initial $[H^+]$	Measured initial rate (mol/L •s)
1	0.10	0.10	0.10	8.0×10^{-4}
2	0.20	0.10	0.10	1.6×10^{-3}
3	0.20	0.20	0.10	3.2×10^{-3}
4	0.10	0.10	0.20	3.2×10^{-3}

A SUMMARY (p.639 in your book)

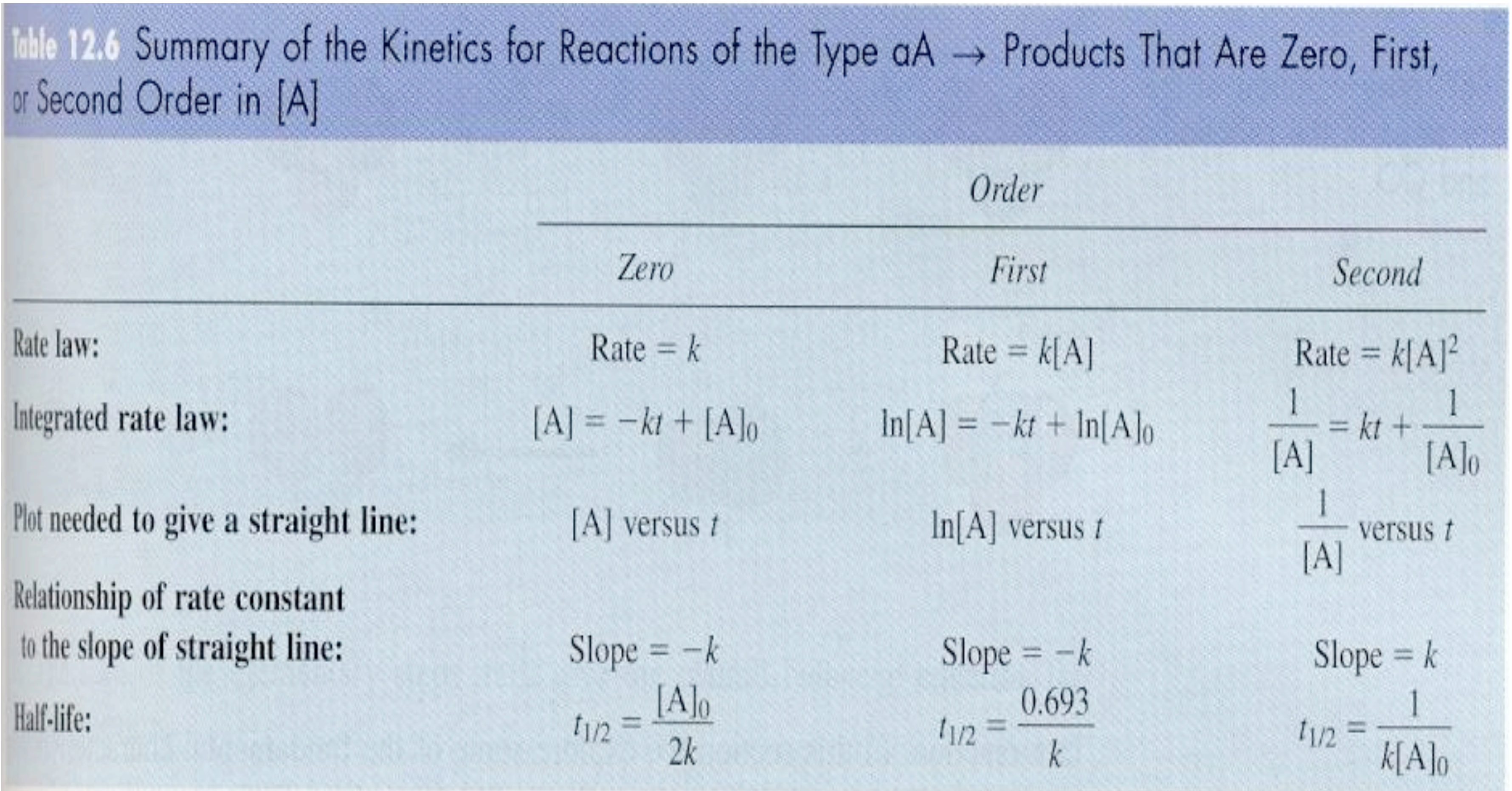


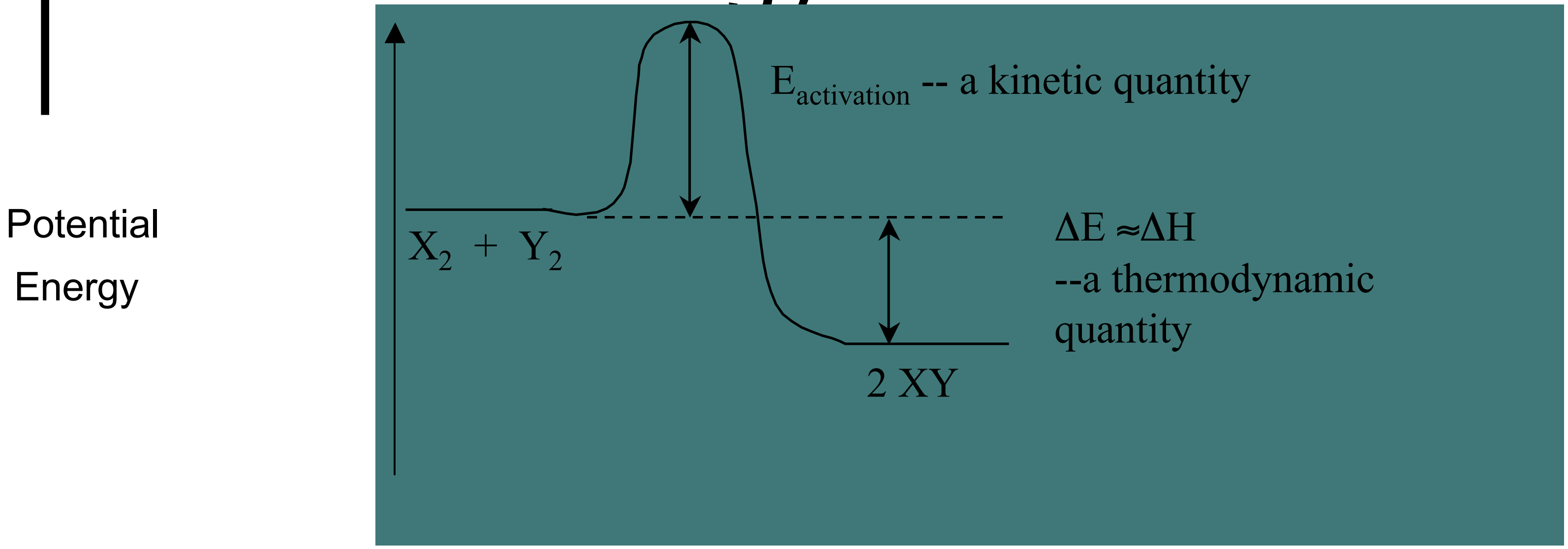
Table 12.6 Summary of the Kinetics for Reactions of the Type aA → Products That Are Zero, First, or Second Order in [A]

	Order		
	Zero	*First*	*Second*
Rate law:	Rate = k	Rate = $k[\mathrm{A}]$	Rate = $k[\mathrm{A}]^2$
Integrated rate law:	$[\mathrm{A}] = -kt + [\mathrm{A}]_0$	$\ln[\mathrm{A}] = -kt + \ln[\mathrm{A}]_0$	$\frac{1}{[\mathrm{A}]} = kt + \frac{1}{[\mathrm{A}]_0}$
Plot needed to give a straight line:	$[\mathrm{A}]$ versus t	$\ln[\mathrm{A}]$ versus t	$\frac{1}{[\mathrm{A}]}$ versus t
Relationship of rate constant to the slope of straight line:	Slope = $-k$	Slope = $-k$	Slope = k
Half-life:	$t_{1/2} = \frac{[\mathrm{A}]_0}{2k}$	$t_{1/2} = \frac{0.693}{k}$	$t_{1/2} = \frac{1}{k[\mathrm{A}]_0}$

Reaction mechanisms again

- What happens if the slow step is NOT the first step?
- Write the rate law for the following reaction from the proposed mechanism.
- $NO_{2(g)} + O_{3(g)} \leftrightarrow NO_{3(g)} + O_{2(g)}$ (fast equilibrium)
- $NO_{3(g)} + NO_{2(g)} \rightarrow N_2O_{5(g)}$ (slow)

Kinetics and net energy of reaction



-relationship between kinetics and thermodynamics

-*endo*thermic—products end up higher in energy than reactants so…. heat is absorbed or taken into or added to the system and given a positive sign.

-*exo*thermic—pictured above, products are of lower energy than reactants so…. heat is lost to the surroundings and given a negative sign.

*Notice in the equation: As "Ea" increases, "k" gets smaller and thus, the rate would decrease.

Also, notice that as "T" goes up, "k" increases and so the rate would also increase.

Applying the laws of logarithms, taking the **natural log of both sides**, ln, we can rewrite the equation:

$$\ln k = \ln A - \frac{Ea}{RT}$$

Rewrite in the form of an equation for a **straight line**, we get:

$$\ln k = -\frac{E_a}{R}\left(\frac{1}{T}\right) + \ln [A]$$

Taking this equation, plot 1/T vs. ln [k], and get a straight line.

From the straight line, find the **slope** and then find the **activation energy.**

$$\text{slope} = -\frac{Ea}{R}$$

so ... $$Ea = -(R)(\text{slope})$$

OR, **find Ea** from data given **mathematically:**

ln =

$$\ln \left(\frac{k_2}{} \right)$$

Used to calculate

-value of activation energy from temperature dependence of the rate constant

-rate constant for a given temp - if the E* [also known as E_a] and A factor are known.

Example - Arrhenius

Calculate the activation energy for the following set of data:

T (°C)	k (l/mol- s)
3	1.4×10^{-3}
13	2.9×10^{-3}
24	6.2×10^{-3}
33	1.2×10^{-2}

Points to remember!!

1. Ea is smaller; k is greater; the reaction is faster.

2. Ea is greater; k is smaller; the reaction is slower.