

Chemical kinetics

- Chemical kinetics area of chemistry concerned with speeds (or rates) of reactions
- Reaction rate the speed at which a reaction occurs
- Rate at which amount of reactants is converted to products per unit time

















Reaction rates and stoichiometry

- $C_4H_9CI(aq) + H_2O(I) \rightarrow C_4H_9OH(aq) + HCI(aq)$
- Rate of appearance of C_4H_9OH is equal to rate of disappearance of C_4H_9CI
- For every 1 mole of C_4H_9Cl consumed, 1 mole of C_4H_9OH is produced
- $\blacksquare Rate = -\frac{\Delta[C_4H_9Cl]}{\Delta t} = \frac{\Delta[C_4H_9OH]}{\Delta t}$









20	*Rate law e One reacto Determine ra	xample ant te law and rate	constant
	Experiment number	Initial A concentration (M)	Observed initial rate (M/s)
	1	00100	5.4 x 10 ^{.7}
	2	0.0200	2.16 x 10 ⁻⁶
	3	0.0400	8.64 x 10 ⁻⁶



 Determine the rate law and rate constant for the reaction using the following data:

Experiment number	Initial B concentration (M)	Observed initial rate (M/s)
1	0.0050	9.3 x 10 ⁻³
2	00100	3.7 × 10 ⁻²
3	0.0025	2.3 × 10 ⁻³

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Rate law example Two reactants

 Determine the rate law and rate constant using initial reaction rate for the following reaction:

■ 2 NO + 2 $H_2 \rightarrow N_2 + 2 H_2O$

Experiment Number	[NO] (M)	[H ₂] (M)	Initial Rate (M/s)
1	0.10	0.10	1.23×10^{-3}
2	0.10	0.20	2.46×10^{-3}
3	0.20	0.10	4.92×10^{-3}

23	Practice	e 1		
	1. Determi initial re OCI ⁻¹	ine the rate to action rate for + I ⁻ \rightarrow OI ⁻ + C	aw and rate o or the followin I ⁻	constant using ng reaction:
	1.5×10^{-3}	1.5×10^{-3}	1.36×10^{-4}	-
	3.0×10^{-3}	1.5×10^{-3}	2.72×10^{-4}	
	$1.5 imes 10^{-3}$	$3.0 imes 10^{-3}$	2.72×10^{-4}	

24	Practice 2. Determininitial rec 2 NO	+ 1 the the rate action rate $+ 2 H_2 \rightarrow 1$	e law and e for the for $N_2 + 2 H_2C$	l rate constant usin ollowing reaction:	ıg
	Experiment Number	[NO] (<i>M</i>)	[H ₂] (M)	Initial Rate (M/s)	
	1	0.10	0.10	1.23×10^{-3}	
	1 2	0.10 0.10	0.10	1.23×10^{-3} 2.46×10^{-3}	
	1 2 3	0.10 0.10 0.20	0.10 0.20 0.10	$\begin{array}{c} 1.23 \times 10^{-3} \\ 2.46 \times 10^{-3} \\ 4.92 \times 10^{-3} \end{array}$	

25	*Pract	ice 1.5				
	 Determine the rate law for the following reaction: BrO₃ (aq)+5Br (aq)+6H⁺(aq) → 3Br₂(aq)+3H₂O(I) 					
		Ir	itial concentratio	ns	Rate in	
	Mixture	Ir [BrO ₃] in M	itial concentratio	ns [H ⁺] in M	Rate in M per unit time	
	Mixture	Ir [BrO ₃] in M 0.0050	Itial concentration [Br] in M 0.025	ns [H ⁺] in M 0.030	Rate in M per unit time	
	Mixture A B	Ir [BrO ₃ ⁻] in M 0.0050 0.010	[Br] in M 0.025 0.025	ns [H ⁺] in M 0.030 0.030	Rate in M per unit time 10 20	
	Mixture A B C	Ir [BrO ₃] in M 0.0050 0.010 0.010	itial concentration [Br] in M 0.025 0.025 0.050	[H⁺] in M 0.030 0.030 0.030	Rate in M per unit time 10 20 40	
	Mixture A B C D	Ir [BrO ₃] in M 0.0050 0.010 0.010 0.010	itial concentration [Br] in M 0.025 0.025 0.050 0.050	[H⁺] in M 0.030 0.030 0.030 0.030 0.030	Rate in M per unit time 10 20 40 160	

Experiment Initial [A] (mol L ⁻¹) Initial [B] (mol L ⁻¹) Initial [B] (mol L ⁻¹) Initial rate of formation of C (mol L ⁻¹) 1 0.125 0.375 2.2x10-4 2 0.375 0.375 6.5x10-4	26	Another More cc Determir the reac 2 A + B =	example emplicated the the rate la tion represer > C + D	with diffe d rate lav aw and rate nted below:	erent metho v calc constant for	bc
1 0.125 0.375 2.2x10-4 2 0.375 0.375 6.5x10-4		Experiment	Initial [A] (mol L ^{.1})	Inifial [B] (mol L ⁻¹)	Initial rate of formation of C (mol L ⁻¹ min ⁻¹)	
2 0.375 0.375 6.5x10 ⁻⁴		1	0.125	0.375	2.2×10-4	
	XX	2	0.375	0.375	6.5x10 ⁻⁴	
3 0.750 0.750 2.7x10 ⁻³		3	0.750	0.750	2.7x10 ⁻³	



28	*(Challenge	problem	
	-	Determine th $2NO(g) + Cl_2$	e rate law ar (g) \rightarrow 2NOCI	nd value of k (g)
	Trial	[NO] (mol/L)	[Cl ₂] (mol/L)	$-rac{\Delta [\mathrm{NO}]}{\Delta t}~(\mathrm{mol}\mathrm{L}^{-1}\mathrm{s}^{-1})$
	1	0.10	0.10	0.00300
	2	0.10	0.15	0.00450
NX .	3	0.15	0.10	0.00675





Rate laws tell us...

- Rate or speed of a reaction
- How the reaction rate changes when reactant concentrations are changed
- How rate changes due to temperature changes (because k is dependent on temperature)
- The reactant concentration at any time during the reaction









38	First order reaction Example	
	Time (s)	P (mmHg)
	0	284
	100	220
	150	193
	200	170
\mathbb{N}	250	150
K		

























Elementary reactions

- Reactions take place because of collisions between reactant molecules
- Elementary reactions take place in single step
- Molecularity total number of molecules reacting in one step



- Termolecular requires three molecules, rate is 3rd order
 - Almost never heard of because the chances of three molecules coming into contact at same time with correct orientation and energy are VERY small





Collision model

- Molecules must collide to react
- Not all collisions result in reactions (actually, only a small fraction do)
 - Molecules must have proper orientation
 - Molecules must have enough energy to react





Collision model Activation energy

- Activation energy minimum energy to initiate chemical reaction
 - Like an energy barrier
 - Colliding molecules must have enough energy to break reactant bonds and create product bonds

























(overall)

(fast)





82	Practice 8 Slow first step	
	3. Write the rate law and ove	erall reaction for:
	Step 1: $N_2O \rightarrow N_2 + O$ Step 2: $N_2O + O \rightarrow N_2 + O_2$	(slow) (fast)

















Practice 10 Multistep reaction energy profile

2. Draw an energy profile that matches the following steps:

Step 1: $NO_2 + F_2 \rightarrow NO_2F + F$ (slow) Step 2: $NO_2 + F \rightarrow NO_2F$ (fast)

(the overall reaction is exothermic)









Catalysis 3 types of catalysts

- Heterogeneous in different phase as reactants
- Homogeneous same phase as reactants
- Biological enzymes







