Chemistry 4B Exam 1

Kshitij Chauhan

TOTAL POINTS

90 / 100

QUESTION 1

N2O5 Decomposition 20 pts

1.1 Calculate Rate Constant **10 / 10**

✓ **+ 10 pts** **Correct Answer with units and sig figs**

+ 0 pts Incorrect

- 2 pts Wrong sig figs or No/wrong units

- 2 pts Calculator Error

+ 2 pts Has integrated first order rate expression

+ 2 pts Plugs in 1/2* original concentration

+ 2 pts Rearranges and solves for k

1.2 Unreacted molecules **10 / 10**

✓ **+ 10 pts** **Correct answer**

+ 2 pts Writes out first order integrated rate expression

+ 2 pts Converts 1 day into seconds (86,400)

+ 2 pts Sets up equation to solve for unreacted molecules

- 2 pts Click here to replace this description.

+ 0 pts no points

QUESTION 2

Pyridine 20 pts

2.1 Diff Rate Expression **10 / 10**

✓ **+ 10 pts** **correct differential rate law by using method of initial rates**

+ 3 pts Writes differential rate law with variables in exponent

+ 2 pts Sets up ratio of rate expressions and solves for order of CH3I

+ 2 pts Sets up ratio of rate expressions to solve for order of C5H4N

+ 0 pts Incorrect

- 3 pts Did not show all work

2.2 Rate Constant **10 / 10**

✓ **+ 10 pts** **Correct answer with units and sig figs**

+ 2 pts Writes correct differential rate equation with orders calculated in part a

+ 2 pts Rearranges and solves for k

+ 2 pts Plugs in correct values from any trial

- 2 pts Wrong sig figs or wrong/no units

- 2 pts Calculation or scientific notation error

+ 0 pts Incorrect or blank

QUESTION 3

Iodine 10 pts

3.1 Calculate Concentration **10 / 10**

✓ **+ 10 pts** **Correct concentration with sig figs and units**

+ 2 pts Writes second order integrated rate law

+ 2 pts Plugs in correct values

- 2 pts Wrong sig figs or wrong / no units

+ 0 pts Wrong integrated rate law

- 2 pts Minor calculation error

- 2 pts Contested rubric (no scoring error)

QUESTION 4

Isomerization Reaction 20 pts

4.1 Calculate Arrhenius Factor **8 / 10**

✓ **+ 10 pts** **Correct answer with units**

+ 2 pts Writes arrhenius equation

+ 2 pts Rearranges and solves for A

+ 2 pts Converts kJ to J or vice versa

✓ **- 2 pts** **Wrong/no units**

+ 0 pts Incorrect

4.2 Calculate Rate Constant **10 / 10**

✓ **+ 10 pts** **Correct final k with units**

- **- 2 pts** wrong sig figs or wrong / no units
- **+ 7 pts** Right calculation with wrong numbers
- **+ 7 pts** Right calculation, arithmetic error
- **- 2 pts** Rounding error
- **+ 8 pts** Right calculation, k not evaluated
- **+ 0 pts** No credit

QUESTION 5

Steady State Assumption 15 pts

5.1 Rate Expression **15 / 15**

- ✓ **+ 15 pts** **Correct answer using steady state approx**
- **+ 3 pts** Starts with correct differential rate law
- **+ 3 pts** Sets up steady state approx
- **+ 3 pts** Solves for [Cl] in ss correctly
- **+ 0 pts** Incorrect
- **- 3 pts** Arithmetic Error / Missing Line
- **- 2 pts** Erroneous Superfluous Information

QUESTION 6

MM Kinetics 15 pts

6.1 Determine Constant **7 / 15**

- ✓ **+ 7 pts** **Correct value for k2 with units and sig figs**
- **+ 8 pts** Correct value for km with unit and sig figs
- **+ 2 pts** Writes MM rate law
- **+ 3 pts** Simplifies rate for high [S]
- **+ 3 pts** Sets up ratio of rates to solve for km
- **- 2 pts** Wrong sig figs or no / wrong units
- **+ 0 pts** incorrect
- **- 2 pts** Small calculation error
- **- 2 pts** Contested the rubric and not a grading error

Chemistry 4B Exam 1
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Equations:

$$c = c_0 e^{-kt}$$

$$\frac{d[P]}{dt} = \frac{k_2[E]_0[S]}{[S] + K_m}$$

$$\frac{1}{c} = \frac{1}{c_0} + 2kt$$

$$A = 2d^2 N_A \sqrt{\frac{\pi RT}{M}} P$$

$$k = A e^{-E_a/RT}$$

Rules:

- Work all problems to ~~**3 significant figures**~~ to correct # of sig figs
- No lecture notes or books permitted
- No word processing, graphing, or programmable calculators
- Time: 50 minutes
- Total: 100 points
- **SHOW ALL WORK IN BOXES PROVIDED TO RECEIVE CREDIT**
- Answers with no work shown will receive no credit
- Periodic Table, Tables of Physical Constants, Equations, and Conversion Factors included

(1) **(20 points)** In lecture we studied the decomposition reaction of N_2O_5:

(a) What is the rate constant, k, for the first-order decomposition of N_2O_5 (g) at 25°C if the half-life of N_2O_5 (g) at that temperature is 4.03×10^4 s ? (10 points)

rate = $k[N_2O_5]$

$t = \frac{\ln 2}{k}$

$k = \frac{\ln 2}{t}$

$k = \frac{\ln 2}{4.03 \times 10^4 \, s}$

$k = 1.72 \times 10^{-5} \, s^{-1}$

(b) What percentage of N_2O_5 molecules will not have reacted after 1 day? (10 points)

$c = c_0 e^{-kt}$

$\frac{c}{c_0} = e^{-kt}$

$\frac{c}{c_0} = e^{-1.72 \times 10^{-5} \, s^{-1} \times 1\,day \times \frac{24\,hr}{1\,day} \times \frac{60\,min}{1\,h} \times \frac{60\,s}{1\,min}}$

$\frac{c}{c_0} = 0.226 \times 100\% = 22.6\%$ ← percentage remaining

percentage that remain = 22.6% after a day

(2) **(20 points)** In a study of the reaction of pyridine (C_5H_5N) with methyl iodide (CH_3I) in a benzene solution, the following set of initial reaction rates was measured at 25 °C for different initial concentrations of the two reactants:

Reaction	**[C_5H_5N] (mol L-1)**	**[CH_3I] (mol L-1)**	**Rate (mol L-1 s-1)**
1	1.00×10^{-4}	1.00×10^{-4}	7.50×10^{-7}
2	2.00×10^{-4}	2.00×10^{-4}	3.00×10^{-6}
3	2.00×10^{-4}	4.00×10^{-4}	6.00×10^{-6}

a) Write the differential rate expression for this reaction. *Show all work.* (10 points)

rate = k[C5H5N]^m [CH3I]^n

$\frac{6.00\times10^{-6}\ mol\ L^{-1}s^{-1}}{3.00\times10^{-6}\ mol\ L^{-1}s^{-1}} = \frac{k(2.00\times10^{-4}\ \frac{mol}{L})^m(4.00\times10^{-4}\ \frac{mol}{L})^n}{k(2.00\times10^{-4}\ \frac{mol}{L})^m(2.00\times10^{-4}\ \frac{mol}{L})^n}$

$2 = 2^n \Rightarrow n = 1$

$\frac{3.00\times10^{-6}}{7.50\times10^{-7}} = \frac{k(2.00\times10^{-4}\ \frac{mol}{L})^m(2.00\times10^{-4}\ \frac{mol}{L})^n}{k(1.00\times10^{-4}\ \frac{mol}{L})^m(1.00\times10^{-4}\ \frac{mol}{L})^n}$

$4 = 2^m 2^n$

$2 = 2^m \Rightarrow m = 1$ rate = k[C5H5N][CH3I]

b). Calculate the rate constant and give its units. (10 points)

rate = k[C5H5N][CH3I]

$7.50\times10^{-7}\ mol\ L^{-1}s^{-1} = k\ 1.00\times10^{-4}\ \frac{mol}{L} \times 1.00\times10^{-4}\ \frac{mol}{L}$

$k = \frac{7.50\times10^{-7}\ \frac{mol}{L\cdot s}}{1.00\times10^{-4}\ \frac{mol}{L} \times 1.00\times10^{-4}\ \frac{mol}{L}}$

k = 75.0 L mol^-1 s^-1

(3) **(10 points)** At 25°C in CCl_4 solvent, the reaction

$$I + I \rightarrow I_2$$

is second-order in concentration of the iodine atoms. The rate constant k has been measured as 8.2×10^9 L mol^{-1} s^{-1}. Suppose the initial concentration of I atoms is 1.00×10^{-4} M. Calculate their concentration after 2.0×10^{-6} s. (10 points)

rate = k[I]²

k = 8.2×10⁹ L mol⁻¹ s⁻¹

t = 2.0×10⁻⁶ s

1/c = 1/c0 + 2kt

1/c = (1 + 2c0kt)/c0

c = c0 / (1 + 2c0kt)

c = 1.00×10⁻⁴ mol/L / (1 + (2)(1.00×10⁻⁴ mol/L)(2.0×10⁻⁶ s)(8.2×10⁹ L/mol·s))

c = 2.3×10⁻⁵ M

[I] = 2.3×10⁻⁵ M

(4) **(20 points)** The activation energy for the isomerization reaction of CH_3CN

$$CH_3NC \rightarrow CH_3CN$$

is 161 kJ mol-1; the reaction obeys first order kinetics, and the rate constant at 600 K is 0.41 s-1.

(a) Calculate the Arrhenius factor A for this reaction (10 points)

$k = Ae^{-\frac{Ea}{RT}}$

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

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

$A = e^{\ln k + \frac{Ea}{RT}}$

$A = e^{\ln(0.41 s^{-1}) + 161 \frac{kJ}{mol} \times \frac{1000 J}{1 kJ} \times \frac{1}{8.3145 \frac{J}{mol \cdot K} \times 600 K}}$

$A = 4.3 \times 10^{13} L mol^{-1} s^{-1}$

(b) Calculate the rate constant for this reaction at 1000 K. (10 points)

$\ln\left(\frac{k_2}{k_1}\right) = -\frac{Ea}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

$k_2 = k_1 e^{-\frac{Ea}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$

$k_2 = (0.41 s^{-1}) e^{-161 \frac{kJ}{mol} \times \frac{1000 J}{1 kJ} \times \frac{1}{8.3145 \frac{J}{mol \cdot K}} \times \left(\frac{1}{1000} - \frac{1}{600}\right)\frac{1}{K}}$

$k_2 = 1.7 \times 10^{5} s^{-1}$

(5) **(15 points)** The mechanism for decomposition of NO_2Cl is:

$$NO_2Cl \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} NO_2 + Cl$$

$$NO_2Cl + Cl \xrightarrow{k_2} NO_2 + Cl_2$$

By making a steady state approximation for [Cl], express the rate of appearance of Cl_2 in terms of the concentrations of NO_2Cl and NO_2.

$$\frac{d[Cl_2]}{dt} = k_2[NO_2Cl][Cl]$$

Steady state approximation for [Cl]

$$\frac{d[Cl]}{dt} = k_1[NO_2Cl] - k_{-1}[NO_2][Cl] - k_2[NO_2Cl][Cl] = 0$$

$$k_1[NO_2Cl] = (k_{-1}[NO_2] + k_2[NO_2Cl])[Cl]$$

$$[Cl] = \frac{k_1[NO_2Cl]}{k_{-1}[NO_2] + k_2[NO_2Cl]}$$

$$\frac{d[Cl_2]}{dt} = \frac{k_1k_2[NO_2Cl]^2}{k_{-1}[NO_2] + k_2[NO_2Cl]}$$

(6) **(15 points)** The enzyme lysozyme kills certain bacteria by attacking a sugar called *N*-acetylglucosamine (NAG) in their cell walls. At an enzyme concentration of 2.0 x 10^{-6} M, the maximum rate for substrate (NAG) reaction, found at high substrate concentration, is 1 x 10^{-6} mol L^{-1} s^{-1}. The rate is reduced by a factor of 2 when the substrate concentration is reduced to 6.0 x 10^{-6} M. Determine the Michaelis-Menten constant K_m as well as k_2 for lysozyme.

when rate is half of maximum rate

$[S] = K_m$

$K_M = 6.0 \times 10^{-6} M$

When rate is maximum

$\frac{d[P]}{dt} = k_2[E_0]$

$k_2 = \frac{1 \times 10^{-6} \frac{mol}{L \cdot s}}{2.0 \times 10^{-6} \frac{mol}{L}}$

$k_2 = 0.5 s^{-1}$