Title: H_2O_2 Kinetics

Alan Yu*, Harrison, Dante, Joshua, Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, New Brunswick, New Jersey 08901.

Abstract

In this experiment, it was determined that the decomposition of H_2O_2 is dependent on both the catalyst concentration, [I⁻], and the initial concentration of hydrogen peroxide. Both species were found to have an order of one which yielded the overall order to be two. The average k value at 298K was found to be 0.001704 $\frac{1}{Ms}$. For 308K, the fourth trial, k was found to be 0.003555 $\frac{1}{Ms}$. The activation energy of the reaction with the catalyst was found to be 56.1 kJ/mol and the pre-exponential factor was found to be $1.18*10^7$ 1/Ms.

Keywords: Decomposition, catalyst, concentration, overall order.

*To whom correspondence should be addressed.

Introduction

In this experiment, the decomposition of hydrogen peroxide with the help of a catalyst was done. Specifically, the rate reactions and the effect of concentration on the overall rate of reaction. Since this is only for two species, equation 1 is created:

$$\text{Rate} = k[A]^a[B]^b \tag{1}$$

where k is the rate constant, a and b are the orders of the species, and Rate is the rate acquired from the trials. To find the overall order of the reaction, the sum of the orders of the species is calculated. Using the first equation, taking the natural log of both sides, the equation can be simplified to:

$$\ln(\text{Rate}) = \ln(k) + a\ln([A]) + b\ln([B]) \tag{2}$$

Since $\ln(k)$ is independent of the concentration of species, $\ln(k)$ is considered as a constant, and if one concentration of species remains constant between two trials, that term is also considered a constant. This allows for the Rate to be found with the means of plotting. After finding the Rate, the rate constants could be found by rearrangement of equation 1 and plugging in values. Using this new found k constant, the Arrhenius equation is formed.

$$k = Ae^{\frac{-E_a}{RT}} \tag{3}$$

where k is the rate constant, E_a is the activation energy, A is the pre-exponential factor, R is the gas constant, and T is the temperature in K. Rearrangement of this equation can be used to find the activation energy of this reaction and determine the effectiveness of the catalyst.

Methods

This experiment was an online lab experiment that the professor has created.

Results

Table I: Experimental Conditions

Trials	Temp °C	Vol H_2O_2 mL	Vol KI mL	Vol H_2O mL	[H_2O_2] mol/L	[KI] mol/L
1	25	7.5	2.5	15.0	0.2940	0.1000
2	25	7.5	7.5	10.0	0.2940	0.3000
3	25	2.5	7.5	15.0	0.0980	0.3000
4	35	7.5	7.5	10.0	0.2940	0.3000

Pressure (mbar) vs Time (s) for Decomposition of Hydrogen Peroxide with I- Catalyst

Legend:
- Trial 1
- 1.24*x + 40
- Trial 2
- 3.73*x + 40
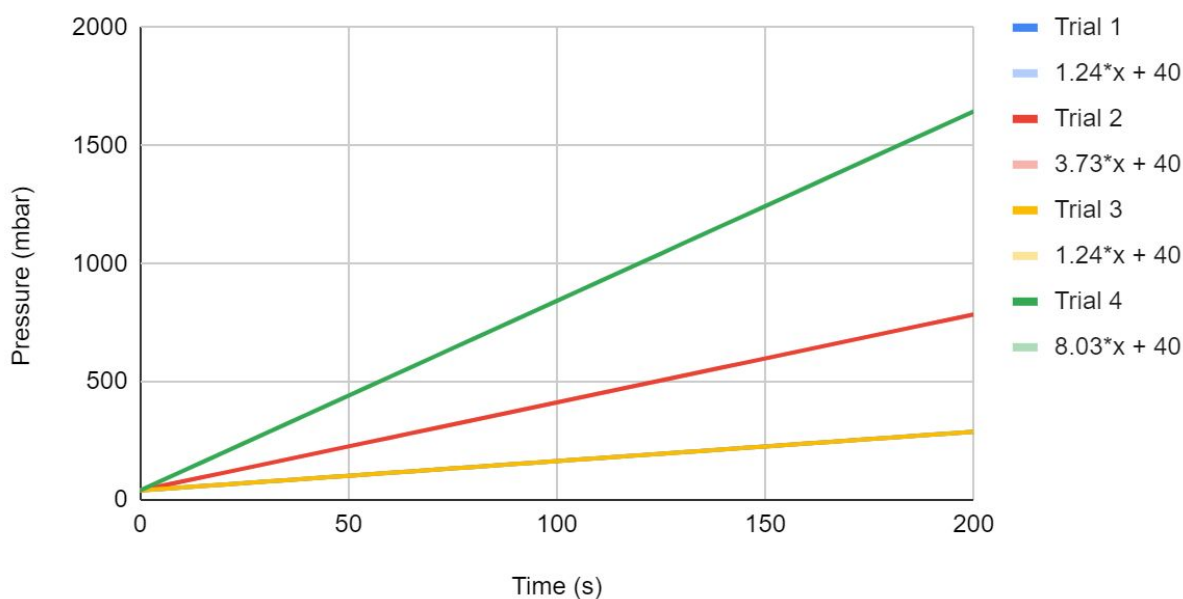- Trial 3
- 1.24*x + 40
- Trial 4
- 8.03*x + 40

Figure 1. Combined graph of all four trials. Note: Trials 1 and 3 are the same, which made them overlap.

Calculations:

Finding rate via slopes of graphs:

Using Figure 1, rates can be converted to SI units:

$$Rate_1 = \frac{1.24\ mbar}{s} * \frac{100\ Pa}{mbar} * \frac{1}{8.3145\frac{J}{mol*K} * 298K} * \frac{1\ m^3}{1000\ L} = 0.00005\frac{mol}{sL}$$

$$Rate_2 = \frac{3.73\ mbar}{s} * \frac{100\ Pa}{mbar} * \frac{1}{8.3145\frac{J}{mol*K} * 298K} * \frac{1\ m^3}{1000\ L} = 0.00015\frac{mol}{sL}$$

$$Rate_3 = \frac{1.24\ mbar}{s} * \frac{100\ Pa}{mbar} * \frac{1}{8.3145\frac{J}{mol*K} * 298K} * \frac{1\ m^3}{1000\ L} = 0.00005\frac{mol}{sL}$$

$$Rate_4 = \frac{8.03\ mbar}{s} * \frac{100\ Pa}{mbar} * \frac{1}{8.3145\frac{J}{mol*K} * 308K} * \frac{1\ m^3}{1000\ L} = 0.00031\frac{mol}{sL}$$

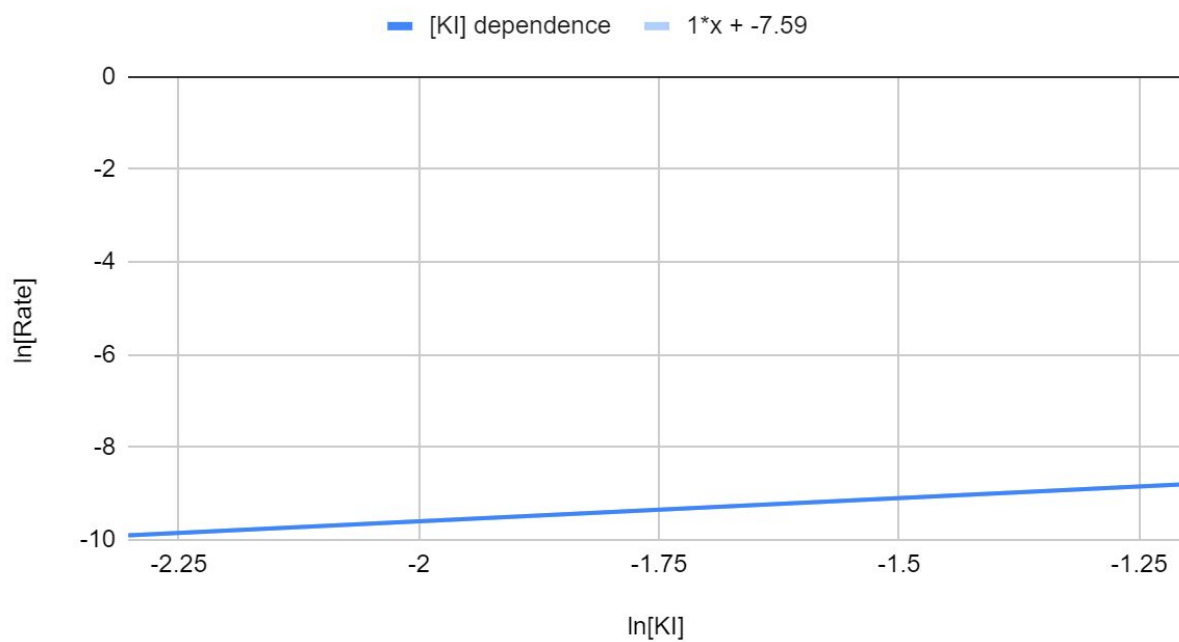Finding a and b from slopes:

ln[Rate] vs ln[KI]

Figure 2. [KI] dependence yielding the order of species in the rate equation.
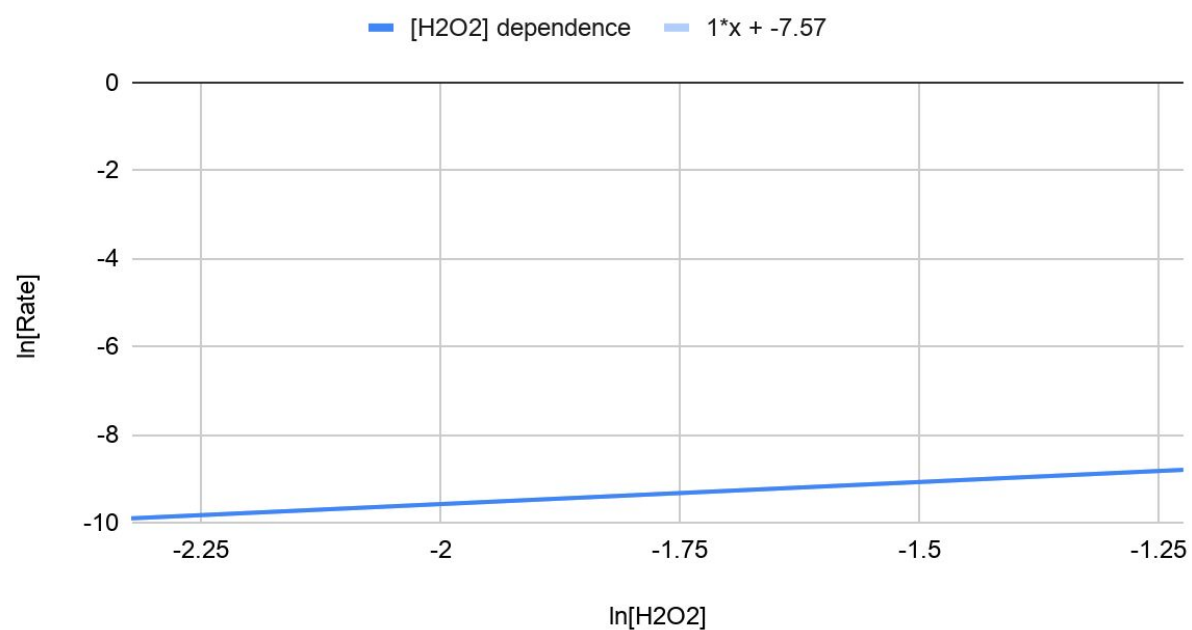
ln[Rate] vs ln[H2O2]

Figure 3. [H_2O_2] dependence yielding the order of species in the rate equation.

From figures 2 and 3, it can be seen that both a and b are first order which makes the overall reaction second order.

To find k, by manipulating equation 1:

$$k_1 = \frac{0.00005\frac{mol}{sL}}{[0.2940M]^1[0.1000M]^1} = 0.001702\frac{1}{Ms}$$

$$k_2 = \frac{0.00015\frac{mol}{sL}}{[0.2940M]^1[0.3000M]^1} = 0.001707\frac{1}{Ms}$$

$$k_3 = \frac{0.00005\frac{mol}{sL}}{[0.0980M]^1[0.3000M]^1} = 0.001702\frac{1}{Ms}$$

$$k_4 = \frac{0.00031\frac{mol}{sL}}{[0.2940M]^1[0.3000M]^1} = 0.003555\frac{1}{Ms}$$

Using trials 1, 2, and 3 to find average k at room temperature:

$$k_{ave} = \frac{k_1+k_2+k_3}{3} = \frac{0.001702\frac{1}{Ms}+0.001707\frac{1}{Ms}+0.001702\frac{1}{Ms}}{3} = 0.001704\frac{1}{Ms}$$

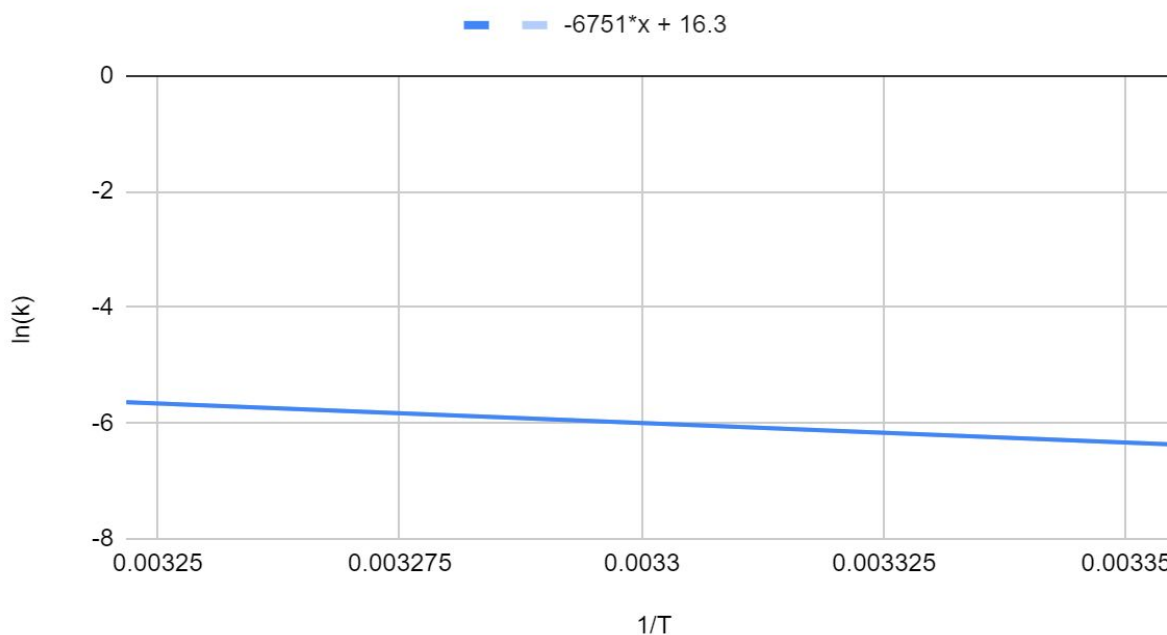Finding the activation energy, figure 4 is created:

Figure 4. Plot of ln(k) vs 1/T to find the slope being $\frac{-E_a}{R}$.

Using the slope of -6751K, multiply by -R to get the activation energy:

$$-6751K \ast 8.3145\frac{J}{K \ast mol} = 56,131\frac{J}{mol} = 56.1\frac{kJ}{mol}$$

Using the activation energy, the pre-exponential factor, A, can be calculated:

$$k = Ae^{\frac{-E_a}{RT}} \rightarrow A = \frac{k}{e^{\frac{-E_a}{RT}}} = \frac{0.001704\frac{1}{Ms}}{e^{\frac{-56,131\frac{J}{mol}}{8.3145\frac{J}{K \ast mol}\ast298K}}} = 1.18 \ast 10^7\frac{1}{Ms}$$

Conclusion

From this experiment, the decomposition rate of hydrogen peroxide with the help of the catalyst potassium iodide was determined. The overall order of the reaction is two, with both compounds having an order of one. This means that both contribute to the rate of decomposition linearly. The rates of the four trials were 0.00005 M/s, 0.00015 M/s, 0.00005 M/s, and 0.00031 M/s respectively. After finding this data, the average k was found for 298K and a k was obtained for 308K being 0.001704 1/Ms and 0.003555 1/Ms respectively. This allowed for the calculation of the activation energy which turned out to be 56.1 kJ/mol. Finally, after finding the activation energy, the pre-exponential factor, A, was found to be $1.18*10^7$ 1/Ms.

Acknowledgements

I used the lecture notes, the lab manual and the online lab that the professor provided.

Discussion Questions

1. Determine a, and b, and then round them to the nearest whole number. Show both the rounded, and unrounded numbers. Use the rounded number for the remainder of the calculations.

Both a and b were determined to be 1, where no rounding was required. Check the Results section for the figures that yielded these values.

2. Estimate the value of k at room temperature. That is, show all your k values, and take the average.

The average of k at room temperature was 0.001704 $\frac{1}{Ms}$. See the Results section for the calculations done.

3. Find the activation energy of the reaction.

The activation energy of the reaction was found to be 56.1 kJ/mol. See Results for the calculation of this value.

4. Find the pre-exponential factor A.

The pre-exponential factor was found to be $1.18 * 10^7 \frac{1}{Ms}$. See Results for the calculations.

5. What is the k value at 35C?

The k value at 35C was calculated to be 0.003555 $\frac{1}{Ms}$. See Results for the calculations.

6. For your reaction, what are the units of the rate constant, k and explain why k can have different units for different reactions?

For my reaction, the units of the rate constant was found to be $\frac{1}{Ms}$. The rate constant can have different units for different reactions because the rate constant depends on the orders of the species in the rate equation.

7. Consider the following first order reaction: $H_2O_2 \rightarrow H_2O + \frac{1}{2} O_2$. Notice this is not catalyzed by I^{-1}. If the initial concentration of H_2O_2 is 0.30M and the initial rate of reaction is $1.0*10^{-3}$ M/s, after 50.0s what will the concentration of H_2O_2 be?

Since the initial rate of reaction is $1.0*10^{-3}$ M/s, we can just multiply this by the value of time to get the change in M.

$$1.0*10^{-3} \text{ M/s} * 50s = 0.05M$$

Using this value, we subtract this from the initial concentration to get 0.25M after 50 seconds.

8. Consider Table II and the following reaction A+B→ products. What are the orders of A and B and the overall order of the reaction? Assume the temperature is the same during the experiments.

Table II: Initial conditions for problem 8

Experiment	Initial [A] M	Initial [B] M	Initial Rate M/s
1	0.1	0.3	10^{-2}
2	0.1	0.6	10^{-2}
3	0.2	0.3	$2*10^{-2}$

To find the orders of A and B, use:

$$\frac{Rate_1}{Rate_2} = \frac{Conc_1}{Conc_2}$$

where all other species not being calculated are the same concentration throughout.

For a:

There was no change from experiment 1 to 3 in the concentration of B, so these values are great to use.

$$\frac{0.2M}{0.1M} = 2$$

$$\frac{2*10^{-2} \frac{M}{s}}{10^{-2} \frac{M}{s}} = 2$$

The order with respect to a species is found by the power that makes both sides equal. So here the power is 1, and with respect to a, the order is 1.

For b:

From experiment 1 to 2, there is no change in the concentration of A. Again:

$$\frac{0.6M}{0.3M} = 2$$

$$\frac{10^{-2} \frac{M}{s}}{10^{-2} \frac{M}{s}} = 1$$

The order here is found to be 0, which means that the concentration of B does not change the rate of reaction. This makes the overall order of the reaction to be 1.

References

Professor's lecture notes, lab manual, and the online lab.