Experiment #3

Investigating Temperature Effects on the Rate of a Chemical Reaction

Objective:

Experimentally determine the effect of temperature on the reaction between acetone and iodine in the presence of catalytic hydronium ion. By using the rate equation determined in experiment 2 and the rates of the reaction at four different temperatures it is possible to calculate the energy of activation for the reaction using the Arrhenius equation.

Reaction Rate as a Function of Temperature.

The rate of a chemical reaction depends on the temperature. The effect of temperature shows up in the rate law through changes in the rate constant. In many cases reaction rates double with every ten (10) degree increase in temperature and this is often given as an approximate rule. However, the relationship between the rate and the temperature is often not so straightforward. In order to understand the relationship between reaction rates and temperature let us look briefly at collision theory.

Collision theory assumes that for a reaction to occur the molecules must collide in the correct orientation and with enough energy for a reaction to take place. As temperature increases the molecules have greater kinetic energy, that is, they are moving faster. Increased speed not only increases the number of collisions, it also increases the amount of energy in the collision. Increased collision energy increases the likelihood that a reaction will occur. For example, compare the damage done when two automobiles collide with each moving five miles per hour with the damage done if each automobile is moving at 60 miles per hour.

Every reaction requires a certain minimum collision energy for the molecules to have enough energy to react. This minimum energy is referred to as the activation energy or E_a. If two molecules collide but the collision does not produce at least as much energy as the activation energy, no reaction will occur.

Collision theory states that the rate constant for a chemical reaction is composed of three factors, (1) the absolute number of collisions, Z, between molecules; (2) The fraction of collisions, f, with an energy greater than the activation energy; and (3) the fraction of molecules, p, in which the molecules are in the correct orientation to react.

$$k = Zfp \qquad \text{Equation 1}$$

The absolute number of collisions, Z, increases with temperature. However, it has been shown that at 25°C, the increase in the number of collisions accompanying a 10°C increase in temperature accounts for only about 2% of the increase in the reaction rate. Similarly, while it is important that molecules be in the proper orientation to react when they collide, molecular orientation is independent of temperature. Thus it follows that the major factor controlling reaction rates is the fraction, f, of molecules in the reaction mixture with an energy greater than the activation energy. This factor, f, depends on the absolute temperature. It has been shown that f is related to E_a by the following equation

$$f = e^{-Ea/RT} \qquad \text{Equation 2}$$

where e = 2.718… is the base for natural logarithms; R is the gas constant with a value of 8.314 J/(mol·K) and T is the temperature measured in Kelvin.

By combining Z and p from equation 1 into a single variable, A, one arrives at a mathematical equation that conveniently expresses the temperature dependence of the rate constant on the temperature. This equation, called the Arrhenius equation after its formulator, Swedish chemist, Savante Arrhenius, is stated in equation 3.

$$k = Ae^{-Ea/RT} \qquad \text{Equation 3}$$

It is convenient to restate equation 3 in terms of logarithms.

$$\ln k = (-E_a/R)(1/T) + \ln A \qquad \text{Equation 4}$$

Equation 4 can then be interpreted as a common straight line equation in the form y = mx + b where y = ln k, m = $(-E_a/R)$, x = 1/T, and B = ln A. Thus the activation energy can be determined through graphical analysis of experimental data since a plot of 1/T versus ln k will have a slope of $-E_a/R$.

One can also write the Arrhenius equation in a form that is more useful for calculations by subtracting the Arrhenius equation at one temperature from the equation at a second temperature. The equation then reduces to Equation 5.

$$\ln\left(\frac{k_2}{k_1}\right) = \left(\frac{E_a}{R}\right)\left(\frac{1}{T_1} - \frac{1}{T_2}\right) \qquad \text{Equation 5}$$

Procedure

Use volumes of reagents as listed in Table 1.

Table 1

Trial number	volume of 4.0 M acetone, ml	volume of distilled water, ml	volume of 1.0 M hydrochloric acid, ml	volume of 5.0×10^{-3} M I_2 solution, ml
1	2.0	4.0	2.0	2.0

Trial 1

1. Prepare a water bath using at least a 400 ml beaker. Use enough tap water to ensure that the water level in the beaker is above the level of the mixture in the test tube after all reagents are added. Make sure that the thermometer is suspended in a clamp, reaching half way into the water/ice bath. For trial 1 allow the tap water to reach room temperature.

NOTE: the liquid in a bath beaker, cold or hot, must be stirred with a glass rod throughout the experiment.

2. Prepare the test tubes with reagents as in experiment 2 (last week). Make the two solutions, one containing acetone, water, and acid and the other containing iodine.
Set the two test tubes with the reagents in the water bath, supported in clamps and leave them in the bath for 5 minutes. It is important to maintain the temperature within 0.5^{o}C of the target temperature (if target is 12^{o}C, the temperature should be maintained between 11.5 and 12.5^{o}C).

3. After the equilibration, leave the iodine test tube in the water bath and pour the contents of the other tube into it. Start the stopwatch when half of the acetone/water/acid mixture has been poured into the iodine mixture. Stir briefly and let the mixture react while in the bath, maintaining the temperature within $0.5^{o}C$ of the target temperature.

4. Record the time required for the disappearance of iodine (the moment the solution turns colorless) and calculate the rate of the equation as in experiment 2, rate = initial $[I_2]/t$.

5. Repeat steps 1-4.

Trial 2-4:
Follow the procedure for Trial 1, but change the temperatures according to Table 2. ***Perform each determination twice***.

Table 2

Trial #	**Temperature**
2	$10^{o}C$ lower than trial 1
3	$10^{0}C$ higher than trial 1
4	$20^{o}C$ higher than trial 1

Calculations
You should use a separate sheet for your calculations but calculation sheets should be legible and must be turned in with your lab report.
1. Calculate the reaction rate at each temperature. Remember that rate = initial $[I_2]/t$

2. Calculate the rate constant values for each trial using the calculated rate and x, y and z values from the rate law determined in experiment 2. Calculate the average value for each trial but do not calculate and overall average value.

3. Calculate the ratio for the rate change for each 10 degree temperature change.

4. Determine the activation energy for the reaction investigated in this experiment. Use a graphical analysis of the all necessary data using the Arrhenius equation (Equation 4). Make a plot of 1/T vs. ln k, calculate the slope of the line (= $-E_a/R$), then determine E_a. You may use a **computer or graph paper** for your analysis or you may use Equation 5.

Discussion

Write a brief discussion of your experiment including a concise description of the experiment itself and a brief discussion of your results including the value and the meaning of E_a.

Prelab **Name** ________________________

1. According to collision theory, what three factors govern the effect of temperature on the rate of a chemical reaction?

2. Briefly define activation energy.

3. In your own words describe how one calculates the energy of activation for a reaction.

4. Based on knowledge obtained from this lab and from your lecture textbook, why would you expect the rate of the reaction of acetone with iodine to increase with increasing temperature?

Postlab **Name ____________________________**

1. Nitric oxide was reacted with chlorine to produce nitrosyl chloride according to the following equation:

$$2NO(g) + Cl_2(g) \rightarrow 2NOCl(g)$$

The rate constant for this reaction at 25^oC is 4.9 X 10^{-6} L/(mol·s) while the rate constant at 35^oC is 1.5 X 10^{-5} L/(mol·s). Use this data to calculate the energy of activation for this reaction.

2. What is the rate constant at 150^oC for the reaction in question 1?

3. Does the reaction between acetone and iodine follow the general rule concerning the relation between a 10-degree increase in temperature and the reaction rate? Explain.

4. What effect does acid have on the rate of the reaction between acetone and iodine? Hint: what is its function?