

THE IODINATION OF ACETONE

Part Two: Determining the Activation Energy for a Chemical Reaction

The rate of a chemical reaction depends on several factors: the nature of the reaction, the concentrations of the reactants, the temperature, and the presence of a possible catalyst. In Part One of this experiment you determined the rate law for a reaction. You will use the rate law from Part One in Part Two, where we will explore the relation between the rate constant and temperature to discover the activation energy for this reaction.

In this experiment you will study the rate of the reaction at different temperatures to find its **activation energy**, E_a . The temperature at which the reaction occurs influences the rate of the reaction. An increase in temperature increases the rate.

As with concentration, there is a quantitative relation between reaction rate and temperature, but here the relation is somewhat more complicated. This relation is based on the idea that to react, the reactant species must have a certain minimum amount of energy present (and the correct geometry, if appropriate) at the time the reactants collide in the reaction step.

This amount of energy, which is typically furnished by the kinetic energy of the species present, is called the **activation energy** (E_a , also known as the *energy of activation*) for the reaction. The formula (called the *Arrhenius equation*) relating the rate constant k to absolute Kelvin temperature T and E_a is:

$$\ln k = \frac{-E_a}{RT} + \ln A$$

In this equation, R is the gas constant (8.314 J/mole K), and natural logarithms (**ln**) need to be used (do not use base 10 logs!) The quantity A is referred to as the **collision frequency** and A can be used to determine the fraction of molecules present with sufficient energy and geometry to become products at a given instant in time.

By measuring k at different temperatures, we can graphically determine the activation energy for a reaction. In this experiment you will determine the effect of temperature on rate and calculate the activation energy for the reaction.

Procedure: *Finding the activation energy*

Using the mixture in experiment #1 in Part One from last time, measure the rate of the reaction at five temperatures over the range of 15 °C to 60 °C, keeping the temperatures at least 5 °C apart. The *only* condition that should be varied in this experiment is the temperature; keep all reactant concentrations identical. You only need to perform each reaction once at each temperature point unless you are not satisfied with a reaction.

Record the **temperature** of the reaction and the **time required** (in seconds) to complete the reaction. At the end you should have five sets of data, and each set should have two pieces of information - time and temperature.

Calculations:

1. Convert your temperatures from °C to K, then take the *inverse* of your Kelvin temperatures.

Example: Convert 37.5 °C to an inverse Kelvin temperature.

Solution: 37.5 °C = 310.7 K. To find the inverse, calculate $(310.7 \text{ K})^{-1} = 3.219 * 10^{-3} \text{ K}^{-1}$

2. Determine the value of the rate constant, k , for each temperature. Find the value of $\ln k$ for each of your rate constant values. *Hint:* use the rate expression determined in last week's lab to calculate k . Remember that the orders of reaction do not change with temperature; only the value of k changes with temperature.

You should have five values of $\ln k$ that correspond with the five temperatures in step 1, above.

Example: Find the value of $\ln k$ for experiment #1 if $k = 2.6 * 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$.

Solution: Remember to use the natural log ("ln") and not the base 10 log ("log") on your calculator. So:

$$\ln k = \ln (2.6 * 10^{-5}) = \mathbf{-10.56}$$

3. Construct a graph of your $\ln k$ values versus the inverse Kelvin temperature values. Make the graph at least as big as half a sheet of paper, and be sure to include unit labels ($\ln k$ for the y-axis and $(\text{Temperature})^{-1}$ for the x-axis).

The data points on your graph should correspond roughly to a straight line with a negative slope. This is the behavior predicted by the Arrhenius equation

$$\ln k = \frac{-E_a}{RT} + \ln A$$

where $\ln k$ is the y-axis, $(\text{Temperature})^{-1}$ is the x-axis, $-E_a/R$ is the slope, $R = 8.3145 \text{ J K}^{-1} \text{ mol}^{-1}$ (the gas constant), E_a is the energy of activation, and A is the collision frequency.

4. Using linear regression on your calculator or Microsoft Excel, use the Arrhenius equation to find the activation energy, E_a . For the x-axis, use the $(\text{Temperature})^{-1}$ values, and for the y-axis use the $\ln k$ values. Report the values of the **slope**, **y-intercept** and **correlation coefficient (r)**.

5. From the value of the slope determined through linear regression, calculate the activation energy. The value of E_a will equal $-\mathbf{R * slope}$.

6. From the value of the y-intercept, calculate the collision frequency, A . The value of A will equal $\mathbf{e^{y-intercept}}$ where e is the anti natural logarithm.

POSTLAB QUESTION: The following reaction was studied at several temperatures, and the following values of k were obtained. Using linear regression, calculate the activation energy for this reaction. Include a graph of $\ln k$ versus $(T)^{-1}$

$2 \text{ N}_2\text{O}_{5(\text{g})} \rightarrow 4 \text{ NO}_{2(\text{g})} + \text{ O}_{2(\text{g})}$	
<u>k (s^{-1})</u>	<u>T ($^{\circ}\text{C}$)</u>
$2.0 * 10^{-5}$	20.0
$7.3 * 10^{-5}$	30.0
$2.7 * 10^{-4}$	40.0
$9.1 * 10^{-4}$	50.0
$2.9 * 10^{-3}$	60.0