Activation Energy

Name________________________________ Lab Section______________________

Log on to the Internet. Type the following address into the location-input line of your browser:

http://cheminfo.chem.ou.edu/~mra/CCLI2004/KR2BN.htm

This will load a Graphics Simulation. Once you have the simulation running your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

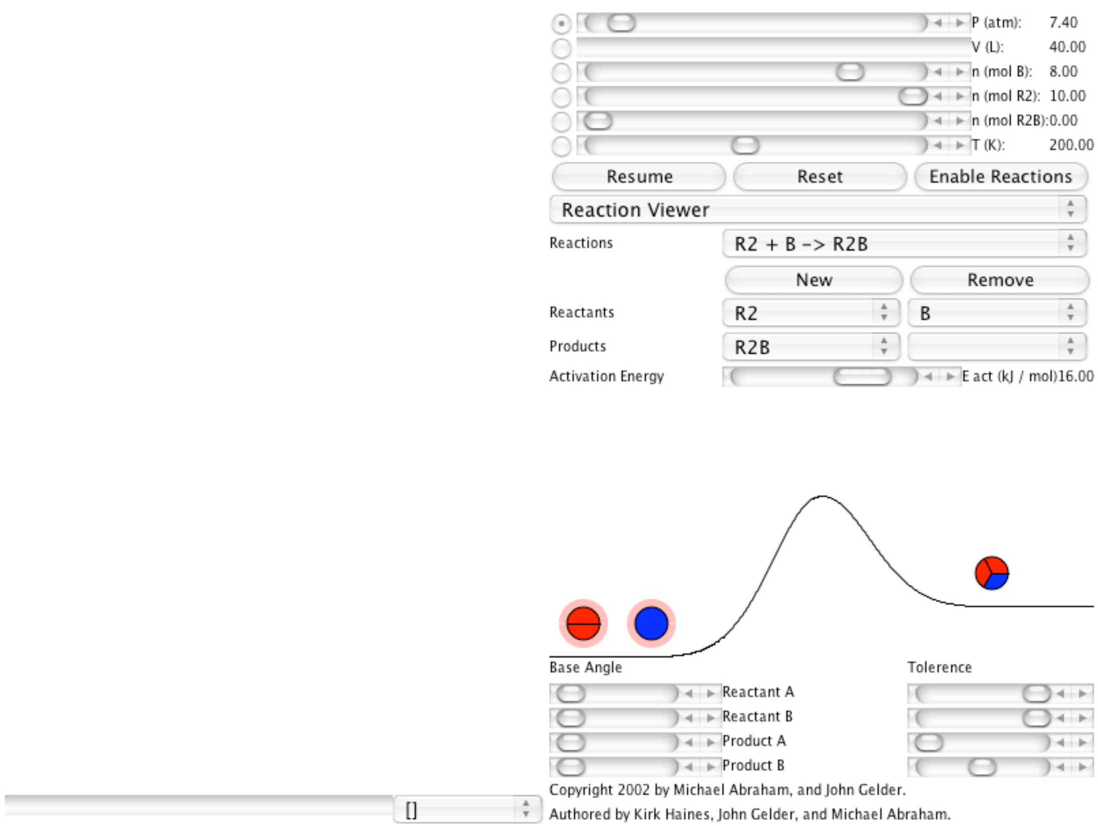

Figure 1

Problem Statement: How does the activation energy affect a chemical reaction?

I. Data Collection:

Open the graphic simulation KR2BN:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/KR2BN.htm

A. Use the information in the simulation to write an equation representing the hypothetical reaction being studied in this activity.

B. Sketch the reaction profile (reaction energy diagram) illustrated in the simulation. Label the sketch using the following terms: potential energy, reactants, products, reaction progress, activation energy, enthalpy, and collision energy. Determine values for the activation energy and enthalpy and include them in your diagram (since the activation energy is known, you can use proportions to estimate enthalpy).

C. Calibrate the time axis (x-axis) of the Strip Chart. To do this, click on the Resume button and with a stopwatch time how long it takes for the strip chart line to proceed across the graphing space. Measure the length of the line in millimeters (mm) with a ruler. Record your data in the spaces below. Do this two more times and calculate an average. Use the average to develop a formula for converting mm to seconds.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

Formula: 1mm = _______seconds

D. In the table below record the beginning concentrations of the reactants and products of the hypothetical reaction you are studying. Click on the Reset button. Click on the Enable Reactions button and the Resume button to begin the reaction. Allow the strip chart to proceed about one half of the way across the Strip Chart Region. Pause the reaction. Record the final concentrations and determine the elapsed time. Calculate the change in concentration and average rate during the elapsed time.

	$[R_2]$	[B]	$[R_2B]$
Initial []			
Final []			
Δ[]			
Time (sec)			
Average Rate			

E. Click on the Reset button. Assume that the hypothetical reaction you are studying has a different activation energy than the one you measured in section I. B. (Remember the reaction profile for a real chemical reaction cannot be adjusted without changing its mechanism. This simulation is only allowing a change in the activation energy to study the affect that activation energy has on the rate of chemical reactions.) Lower the activation energy by 2 kJ/mol and repeat the procedure of the previous section.

	$[R_2]$	[B]	$[R_2B]$
Initial			
Final			
Δ[]			
Time (sec)			
Average Rate			

F. Click on the Reset button. Lower the activation energy by another 2 kJ/mol and repeat the procedure of the previous section. (The easiest way to return the simulation to its default state if you have to start over is to use the refresh button of your browser to reload the software.)

	$[R_2]$	[B]	$[R_2B]$
Initial			
Final			
Δ[]			
Time (sec)			
Average Rate			

II. Data Analysis and Interpretation:

A. What happens to the rate of a chemical reaction that has a lower activation energy? Use both the strip chart graph and your data points as evidence for your conclusion.

B. Explain why a lower activation energy has that effect?

III. Data Collection:

Open the graphic simulation KR2GN:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/KR2GN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

C. Turn your attention to the Reaction Viewer. Use the Reactions pull down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

D. Sketch out the reaction profiles for each of the steps in the reaction mechanism. Label each of the profiles as you did in section I.B.

E. Click on the Reset button. Remove the Tolerence halo from the product molecule in the first step of the mechanism. (This is so that no reverse reaction can take place.) Adjust the amounts of the reactants and products so that you have only 5 moles of the reactant of the first step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Resume and then the Enable Reactions buttons to begin the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

F. Click on the Reset button. In the drop down menu in the Module Control Region select Kinetics. Adjust the amounts of the reactants and products so that you have only 5 moles of the reactant of the first step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the step you are studying to estimate the rate of that step.

G. In the drop down menu in the Module Control Region select Reaction Viewer. Click on the Reset button. Display the second step of the mechanism. Adjust the amounts of the reactants and products so that you have only 5 and 4 moles of the reactants of the second step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Resume and then on the Enable Reactions buttons to begin the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

H. Click on the Reset button. In the drop down menu in the Module Control Region select Kinetics. Adjust the amounts of the reactants and products so that you have only 5 and 4 moles of the reactants of the second step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the step you are studying to estimate the rate of that step.

IV. Data Analysis and Interpretation:

Compare the rates of the two steps of the mechanism for the reaction. Why is one of the steps slower than the other? How are the rates of the steps related to the reaction profiles?

V. Data Collection:

Use the refresh button of your browser to restore the simulation to its original form. Click on the Reset button. In the drop down menu in the Module Control Region select Kinetics. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the overall reaction to calculate the rate of the reaction.

VI. Data Analysis and Interpretation:

A. Compare the rate of the overall reaction with the rates of the individual steps in the mechanism. (See sections III. F. and H.)

B. What conclusion can you draw concerning the role that each step in a mechanism plays in the rate of a chemical reaction?

VII. Data Collection:

Design experiments to investigate the relationship between the rate of production of the product R_2G and the initial concentrations of the reactants of the reaction you are studying. Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[ ]	[ ]	Initial Rate, $\Delta[R_2G]/\Delta time$

VIII. Data Analysis and Interpretation:

A. What effect does doubling the concentration of G have on the initial rate of the reaction?

B. What effect does doubling the concentration of R have on the initial rate of the reaction?

C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants R and G (see section IV.A.). Determine the rate constant for the reaction.

IX. Data Collection:

Open the graphic simulation KB2RN:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/KB2RN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Turn your attention to the Reaction Viewer. Use the Reactions pull down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

C. Design experiments to investigate the relationship between the rate of production of the product B_2R and the initial concentrations of the reactants of the reaction you are studying. Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[ ]	[ ]	Initial Rate, $\Delta[B_2R]/\Delta time$

X. Data Analysis and Interpretation:

A. What effect does doubling the concentration of B have on the initial rate of the reaction?

B. What effect does doubling the concentration of R have on the initial rate of the reaction?

C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants B and R. Determine the rate constant for the reaction.

D. How would you characterize each step in the mechanism in terms of the number of the original reactant particles necessary for the stoichiometry of the reaction? How is this related to the rate law you proposed in section XI.?

E. How would you characterize the number and kind of reactant particles necessary to determine the rate of the overall reaction? How does the mechanism explain why each reactant particle is necessary or not necessary to determine the rate?

F. Compare the rate laws for the reaction KR2GN with the reaction KB2RN. What are the differences in the mechanisms of the reactions that accounts for the differences in the rate laws?