Mechanisms of a Chemical Reaction

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/KRGBM.htm

This will load a Particulate 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 Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

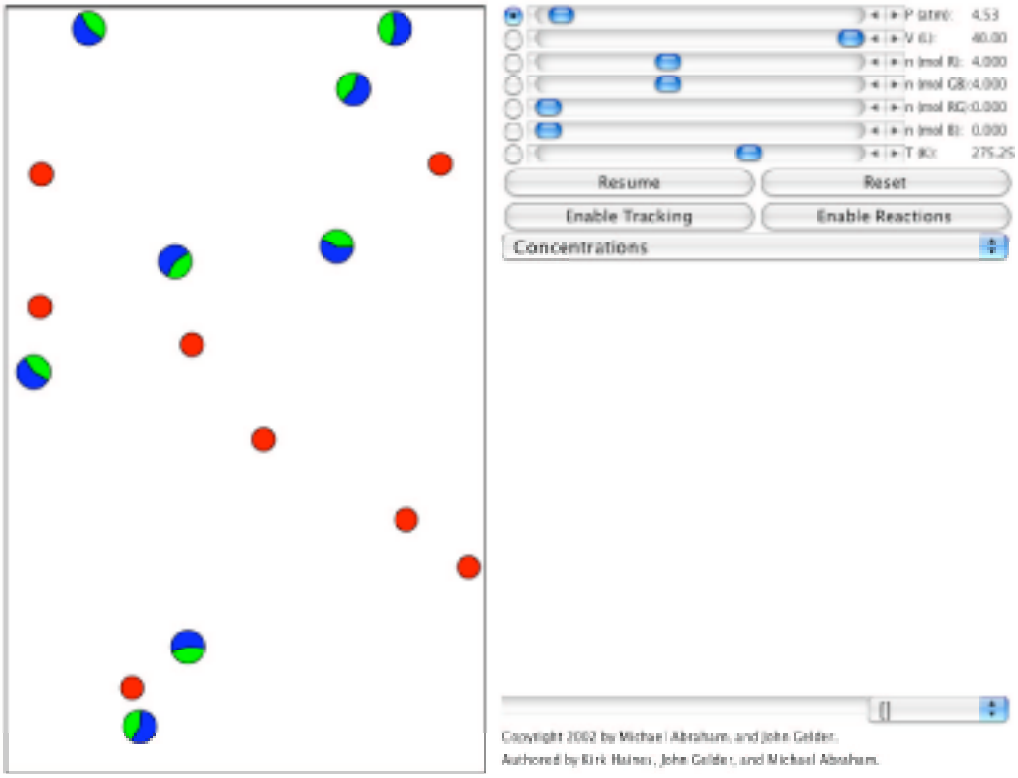

Figure 1.

Problem Statement: How does a chemical reaction proceed from reactants to products?

I. Data Collection:

Open the molecular simulation KRGBM:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/KRGBM.htm

A. Based on what you observe in the sample region and control bar region of the screen, record the number and the concentration of R, BG, B, and RG particles in the table below.

	R	BG	B	RG
# of Particles				
Concentration (M)				

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Record your observations of what is happening. Use some or all of the following terms in your description: atom, molecule, particle, collision, effective collision, speed, energy, orientation, reactants, and products.

C. Allow the simulation to run until no more changes occur. Click on the Pause button and record your observations. Record the number and concentration of each kind of particle.

	R	BG	B	RG
# of Particles				
Concentration (M)				

II. Data Analysis and Interpretation:

A. Write a balanced equation for the reaction you have observed in this simulation.

B. Draw and label the appearance of the strip chart. Identify each kind of particle on the strip chart and explain what is happening to each over time.

C. What criteria did you use to decide the reaction was finished?

III. Data Collection:

Reset the simulation. Then click on the Resume and Enable Reactions buttons. Systematically observe multiple collisions between each of the possible combinations of pairs of the reactant and product particles (see the table below). Note when pairs of collisions result in a change. Use the following table to guide and record your observations. In order to aid your observations you can do the following: (a) change the amounts of the reactant and product particles, (b) use the Enable Tracking button with different particles, (c) use the replay option, (d) change the volume of the container, and (e) change the temperature of the sample.

Collisions Between					
Particle 1	Particle 2	Result	Speed	Orientation	Comments
R	R	No reaction	--	--	--
R	BG				
R	B				
R	RG				
BG	B				
BG	BG				
BG	RG				
B	B				
B	RG				
RG	RG				

IV. Data Analysis and Interpretation:

A. Use the data from the table to write a balanced equation to represent your observations. Compare this equation with the one you wrote for section IIA.

B. Even those collisions between particles that can result in a change don't do so 100% of the time. From your observations can you propose at least two different reasons why some collisions result in a change and others don't.

V. Conclusions:

In the boxes below draw pictures showing how a possible collision between reactant molecules might form product molecules for the KRGBM reaction. Make sure the orientation of the collision supports the arrangement of the atoms in the reactant and product molecules.

Reactants	Collision	Products

VI. Data Collection:

Open the molecular simulation K2GBM:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/K2GBM.htm

A. Based on what you observe in the sample region and control bar region of the screen, record the number and the concentration of R, BG, B, and RG particles in the table below.

	G	B	G_2	GB	G_2B	B_2
# of Particles						
Concentration (M)						

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Record your observations of what is happening.

C. Allow the simulation to run until no more changes occur. Click on the Pause button and record your observations. Record the number and concentration of each kind of particle.

	G	B	G_2	GB	G_2B	B_2
# of Particles						
Concentration (M)						

VII. Data Analysis and Interpretation:

A. Write an overall balanced equation to represent your observations.

B. Draw and label the appearance of the strip chart. Identity each kind of particle on the strip chart and label what is happening to the particles at each change in the chart.

C. What criteria did you use to decide the reaction was finished?

VIII. Data Collection:

A. Use the simulation to design and carry out experiments to explore all of the possible collisions between reactant particles. In order to aid your observations you can do the following: (a) change the amounts of the reactant and product particles, (b) use the Enable Tracking button with different particles, (c) use the replay option, (d) change the volume of the container, and (e) change the temperature of the sample. Use the following table to guide and record your observations.

Reactant 1	Reactant 2	Result	Comments
B	B		
B	G		
G	G		

Describe the experiments you carried out.

Write the chemical equation(s) to summarize the experiments.

B. In a manner similar to section VIII, A. design and carry out additional experiments to explore further all of the possible collisions between the product molecule(s) you identified from section VII. A. with the other reactant particles. Design and construct a table to record your observations.

Describe the experiments you carried out.

Write the chemical equation(s) to summarize the experiments.

IX. Conclusions

A. Using the data you collected in part VIII, propose a step-by-step process (mechanism) showing how the reaction in the molecular simulation K2GBM proceeds from reactants to final products.

B. An alternate possible mechanism for the reaction in the molecular simulation K2GBM is a one step process described by the following: $2G + B \rightarrow G_2B$. Why is this mechanism less likely than the one you proposed?