Extent 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://introchem.chem.okstate.edu/DCICLA/ERGBN.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.

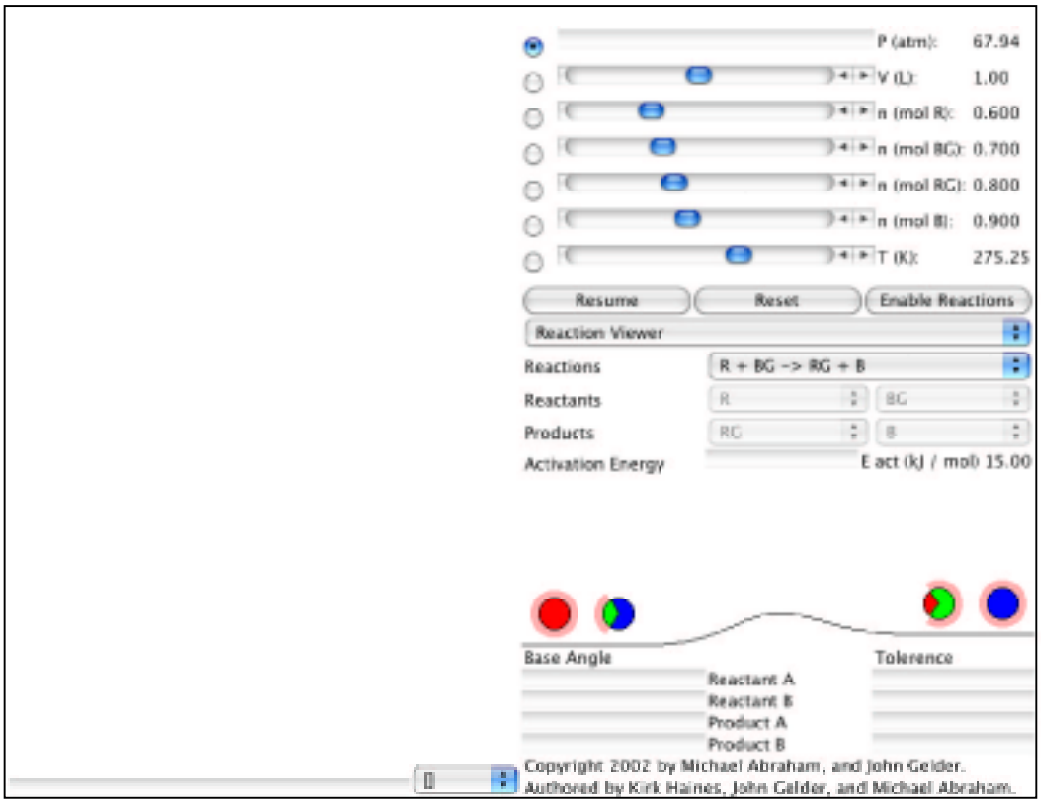

Figure 1.

Problem Statement: What is the relationship between reactant and product concentrations at the end

of a reaction?

I. Data Collection:

Open the Graphic Simulation program for the R + BG reaction. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #1:	R	+ BG →	RG	+ B
Initial Concentration – I	2.0	2.0	0	0
Concentration Change – C	**-1.362**	**-1.362**	**+1.362**	**+1.362**
Ending Concentration – E	**0.638**	**0.638**	**1.362**	**1.362**

Pressure **67.94 atm**

Volume **1.00 L**

Temperature **275.25 K**

II. Data Analysis and Interpretation:

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

The Change row is shown in the table above.

B. Draw and label the appearance of the strip chart. Identity each kind of particle on the strip chart and explain what is happening to each over time. How does the strip chart illustrate the change in the data in the table?

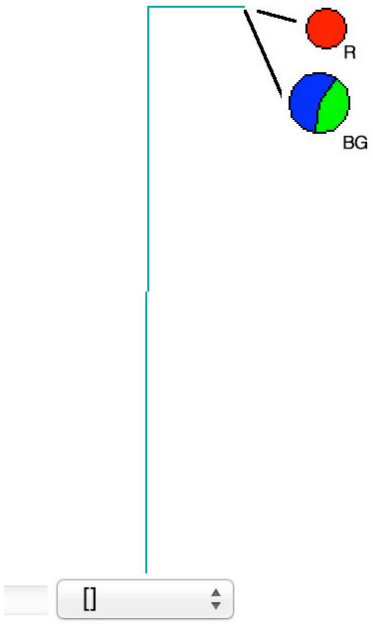

Figure II.

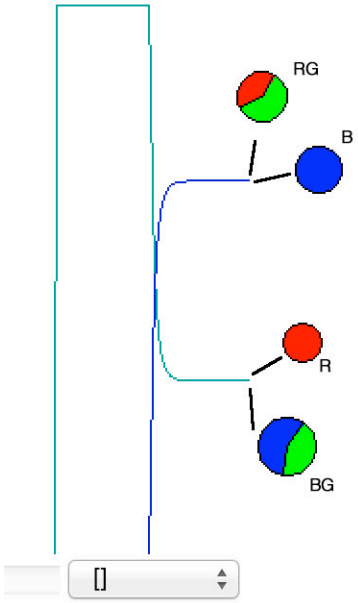

Figure III.

In Figure II the initial amounts of all species is shown. Note that there is one line for the reactants, R and BG, since they are present initially in the same amounts. The Initial amounts are also shown in the ICE table above. When the Enable Reaction button is clicked the reaction occurs until no further change in the amounts of reactants and products. The ICE table shows the final amounts of the reactants and products. Once the Final amounts are obtained the Change amounts can be determined. It is very important to note tat in the Change amounts, the ratio of the amounts of reactants and products reflect the ratio of the coefficients in the balanced chemical equation. This is not the case in the Initial amounts, or in the Final amounts.

III. Data Collection:

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #2:	R +	BG → RG	+ B
Initial Concentration – I	1.0	1.0	0	0
Concentration Change – C	**-0.681**	**-0.681**	**+0.681**	**+0.681**
Ending Concentration – E	**0.319**	**0.319**	**0.681**	**0.681**

Pressure **45.29 atm**

Volume **1 Liter**

Temperature **275.25 K**

IV. Data Analysis and Interpretation:

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

The Change row is shown in the table above.

B. Draw and label the appearance of the strip chart. Identity each kind of particle on the strip chart and explain what is happening to each over time. How does the strip chart illustrate the change in the data in the table?

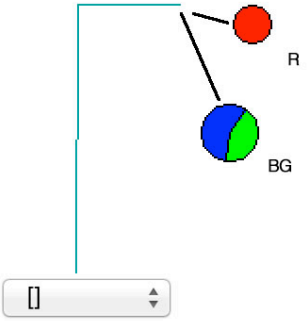

Figure IV.

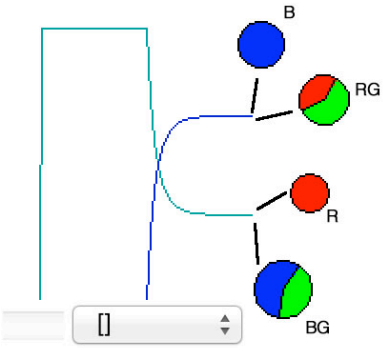

Figure V.

C. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R +	BG → RG +	B
Initial Concentration – I	1.5	1.5	0	0
Predicted Concentration Change – C	**-1.02**	**-1.02**	**+1.02**	**+1.02**
Predicted Ending Concentration – E	**0.48**	**0.48**	**+1.02**	**+1.02**

Since the Initial amounts in Experiment #2 are twice the Initial amounts in Experiment #1, and the amount reacting in Experiment #1 are twice the amounts reacting in Experiment #2, then I assumed in Experiment #3 the amount reacting (the Change row) would be 1.5 times the amount reacting in Experiment #2.

V. Data Collection:

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the

following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #3:	R +	BG → RG +	B
Initial Concentration – I	1.5	1.5	0	0
Concentration Change – C	**-1.02**	**-1.02**	**+1.02**	**+1.02**
Ending Concentration – E	**0.48**	**0.48**	**+1.02**	**+1.02**

Pressure **67.94 atm**

Volume **1 liter**

Temperature **275 K**

VI. Data Analysis and Interpretation:

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

See the Table above.

B. Comment on how your predictions in IV. C. compared to the actual values determined from experiment.

My predictions and the results from running the simulation matched exactly. The experience from Experiments#1 and #2 helped me predict what would happen in Experiment #3.

C. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R +	BG → RG +	B
Initial Concentration – I	0	0	1.0	1.0
Predicted Concentration Change – C	**+0.319**	**+0.319**	**-0.319**	**-0.319**
Predicted Ending Concentration – E	**0.319**	**0.319**	**0.681**	**0.681**

NOTE: There will be a subset of students who will predict the Change amount will be;

Predicted Concentration Change – C	**+0.681**	**+0.681**	**-0.681**	**-0.681**
Predicted Ending Concentration – E	**0.681**	**0.681**	**0.319**	**0.319**

Watch out for that issue. We cannot address why one is correct and one is wrong, until later in the experiment.

VII. Data Collection:

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #4:	R +	BG → RG +	B
Initial Concentration – I	0	0	1.0	1.0
Concentration Change – C	**+0.319**	**+0.319**	**-0.319**	**-0.319**
Ending Concentration – E	**0.681**	**0.681**	**0.681**	**0.681**

Pressure **45.29 atm**

Volume **1 Liter**

Temperature **275.25 K**

VIII. Data Analysis and Interpretation:

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

See the Table above.

B. Comment on how your predictions in VI. C. compared to the actual values determined from experiment.

Once again my prediction and the results from running the simulation matched exactly. The experience from Experiments #2 helped me predict what would happen in Experiment #4.

C. Compare your data in sections III. (Experiment #2) and VII. (Experiment #4). How do you explain this comparison?

The Final amounts in both Experiment #1 and #4 are the same. Since the Initial amounts are different in whether there are some reactants, or some products the amounts of each is the same. A prediction of Final amounts that are the opposite could also be made in Experiment #4 compared to Experiment #2. At this point it is difficult to explain why one prediction is better (as a prediction).

D. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R	+ BG →	RG	+ B
Initial Concentration – I	2.0	0.5	0	0

Predicted Concentration Change – C	**-0.350**	**-0.350**	**+0.350**	**+0.350**
Predicted Ending Concentration – E	**1.650**	**0.150**	**+0.350**	**+0.350**

For this prediction the reaction has to go from left to right to reach the Final amounts, and the amounts that react must follow the stoichiometry of the balanced chemical equation.

What was observed:

IX. Data Collection:

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #5: R + BG → RG + B

Initial Concentration – I	2.0	0.5	0	0
Concentration Change – C	**-0.469**	**-0.469**	**+0.469**	**+0.469**
Ending Concentration – E	**1.531**	**0.031**	**0.469**	**0.469**

Pressure **56.62 atm**

Volume **1.0 Liters**

Temperature **275 K**

X. Data Analysis and Interpretation:

A. Calculate the change in concentration of each of the particles in the reaction and record the

values in the above table.

B. Comment on how your predictions in VIII. D. compared to the actual values determined from experiment.

The predicted direction of the reaction and the observed direction of the reaction were correct. Also the stoichiometric amounts in the Change row were correct, however the exact amount predicted was not correct. The reaction went further to the right than was predicted.

XI. Data Collection:

A. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations and the change in concentration of each of the particles in the following table.

EXPERIMENT #6:	R	+ BG →	RG	+ B
Initial Concentration – I	1.0	0.6	1.2	0.8
Concentration Change – C	**-0.207**	**-0.207**	**+0.207**	**+0.207**
Ending Concentration – E	**0.793**	**0.393**	**1.407**	**1.007**

Pressure **81.53 atm**

Volume **1.0 Liters**

Temperature **275 K**

B. Carry out two additional experiments by adjusting the concentrations of the reactants and products to values of your choosing. Be careful that the ending concentrations do not try to exceed the limits of the allowable values. Check to make sure the ending values of volume and temperature do not change.

EXPERIMENT #7: R + BG → RG + B

Initial Concentration – I	**1.0**	**1.0**	**1.0**	**1.0**
Concentration Change – C	**-0.362**	**-0.362**	**+0.362**	**+0.362**
Ending Concentration – E	**0.638**	**0.638**	**1.362**	**1.362**

Pressure _____

Volume _____

Temperature _____

EXPERIMENT #8: R + BG → RG + B

Initial Concentration – I	**1.0**	**0.6**	**2.0**	**2.0**
Concentration Change – C	**+0.108**	**+0.108**	**-0.108**	**-0.108**
Ending Concentration – E	**1.108**	**0.708**	**1.892**	**1.892**

Pressure _____

Volume _____

Temperature _____

XII. Data Analysis:

Summarize the ending concentrations of reactants and products for the eight reactions you studied in this activity by recording your data in the left hand sections of the following table.

Pressure _____

Volume ___ ___

Temperature _____

					Calculation Results		
	R + BG → RG + B				$\frac{[R][BG]}{[RG][B]}$	$\frac{[RG][B]}{[R][BG]}$	$\frac{[R][BG]}{[RG][B]}$
Experiment #1-Ending Concentration –E	**0.638**	**0.638**	**1.362**	**1.362**	**0.755**	**4.56**	**0.219**
Experiment #2-Ending Concentration –E	**0.319**	**0.319**	**0.681**	**0.681**	**0.047**	**4.56**	**0.219**
Experiment #3-Ending Concentration –E	**0.479**	**0.479**	**1.021**	**1.021**	**0.239**	**4.56**	**0.219**
Experiment #4-Ending Concentration –E	**0.319**	**0.319**	**0.681**	**0.681**	**0.047**	**4.56**	**0.219**
Experiment #5-Ending Concentration –E	**1.531**	**0.031**	**0.469**	**0.469_**	**0.0104**	**4.63**	**0.216**
Experiment #6-Ending Concentration –E	**0.793**	**0.393**	**1.407**	**1.007**	**0.890**	**4.55**	**0.220**
Experiment #7-Ending Concentration –E	**0.638**	**0.638**	**1.362**	**1.362**	**0.755**	**4.56**	**0.219**
Experiment #8-Ending Concentration –E	**1.108**	**0.708**	**1.892**	**1.892**	**2.81**	**4.56**	**0.219**

XIII. Data Interpretations and Conclusions:

A. What conclusions can be drawn from these data? Find an algebraic equation that relates the actual concentrations of the reactants and products of the reaction studied. (Hint: Try all possible combinations of the four concentrations by multiplication and/or division. For example multiply all four together, multiply two and divide by the other two, etc., looking for the combination that gives the most constant result.) Summarize your results for three possibilities in the table above. Label each column with how you combined the four concentrations in the box provided. Discuss your results below.

Column #1 : [R][BG][RG][B]

Column #2 : $\frac{\textbf{[RG][B]}}{\textbf{[R][BG]}}$

Column #3 : $\frac{\textbf{[R][BG]}}{\textbf{[RG][B]}}$

For Column #2 and #3 the values are the same, a constant (or close to a constant).

B. Use your results to predict the ending concentrations for the following. Show how you made your prediction. Check your prediction with the Graphic Simulation.

Predicting:

We want the ratio to equal 4.56, so try about half of the BG reacting. So Ending amounts would be R = 0.7, BG = RG = B= 0.3. So the ratio would be $\frac{\textbf{[0.3][0.3]}}{\textbf{[0.3][0.7]}}$ **= 0.42. SO this is too small so the reaction needs to go further, so try 0.5 moles of BG reacting, R = 0.5, BG = 0.1, RG = B= 0.5 :** $\frac{\textbf{[0.5][0.5]}}{\textbf{[0.1][0.5]}}$ **= 5**

	R + BG → RG + B			
Initial Concentration – I	1.0	0.6	0	0
Concentration Change – C	**-0.5**	**-0.5**	**+0.5**	**+0.5**

Ending Concentration – E	**0.5**	**0.1**	**+0.5**	**+0.5**

Pressure **36.23 atm**

Volume **1 L**

Temperature **273 K**