Name:_____

PhET Reaction Rates Simulation

Part 1: Reaction Rate and Equilibrium

Go to: http://phet.colorado.edu/en/simulation/reactions-and-rates and click "Run Now!" When the simulation has opened, click on the "Many Collisions" tab.

The reaction you are observing is A + BC → AB + C.

1. Look at the graph on the side of the screen. Is this reaction endothermic or exothermic?_____
2. In the box labeled "Current Amounts" enter 50 for A and 50 for BC. Watch what happens for about 30 seconds.
    a. Describe what happened.

    b. Describe the nature of dynamic equilibrium when only a small number of particles (like 50) are present.

3. What will happen to the chemical reaction taking place when the temperature is raised so it is NOT above the activation energy max but IS above the energy level of the products? Use the "Temperature" box below your collision box, raise the temperature so it matches this scenario. Describe what happens.

4. Now, raise the temperature to the activation energy max. Describe what happens.

5. What did you notice about the rate at which reactants/products fluctuated between the three different temperatures? If you didn't notice anything, hit "reset all" and test it again.

6. Did temperature affect the equilibrium position? Did it affect it in the way you expected? Explain.

7. Did temperature affect reaction rate? Did it affect it in the way you expected? Explain.

8. Write the equilibrium expression for this reaction.

Part 2: LeChatelier's Principle

Click on the "Rate Experiments" tab. You are still observing the same reaction: A + BC → AB + C. In the "Initial Conditions" box, add 80 A's and 80 BC's. Move the "Initial Temperature" so that the "total average energy" is even with the "potential energy" in the graph. Start the experiment and let the reaction run until equilibrium is reached. This could take a couple of minutes.

1. What are your numbers of molecules when your reaction reaches equilibrium?

   A_____ BC_____ AB_____ C_____

2. According the LeChatelier's Principle, what will happen to the equilibrium position when the temperature is raise? What will happen when the temperature is lowered?

3. Using the "Temperature" box, raise the temperature of this reaction to above the activation energy max. What happens to the equilibrium of this reaction? Use numerical data to support your explanation.
4. Using the "Temperature" box, lower the temperature of this reaction below the potential energy. What happens to the equilibrium of this reaction? Use numerical data to support your explanation.

Click the "End Experiment" button. You are still observing the same reaction: A + BC → AB + C. In the "Initial Conditions" box, add 50 A's and 80 BC's. Move the "Initial Temperature" so that the "total average energy" is even with the "potential energy" in the graph. Start the experiment and let the reaction run until equilibrium is reached. This could take a couple of minutes.

1. What are your numbers of molecules when your reaction reaches equilibrium?

   A_____ BC_____ AB_____ C_____

2. Why did the equilibrium change when we added more BC?

3. Assuming this reaction is taking place in the gas phase, what would be the effect on the equilibrium position of decreasing the volume of the container?

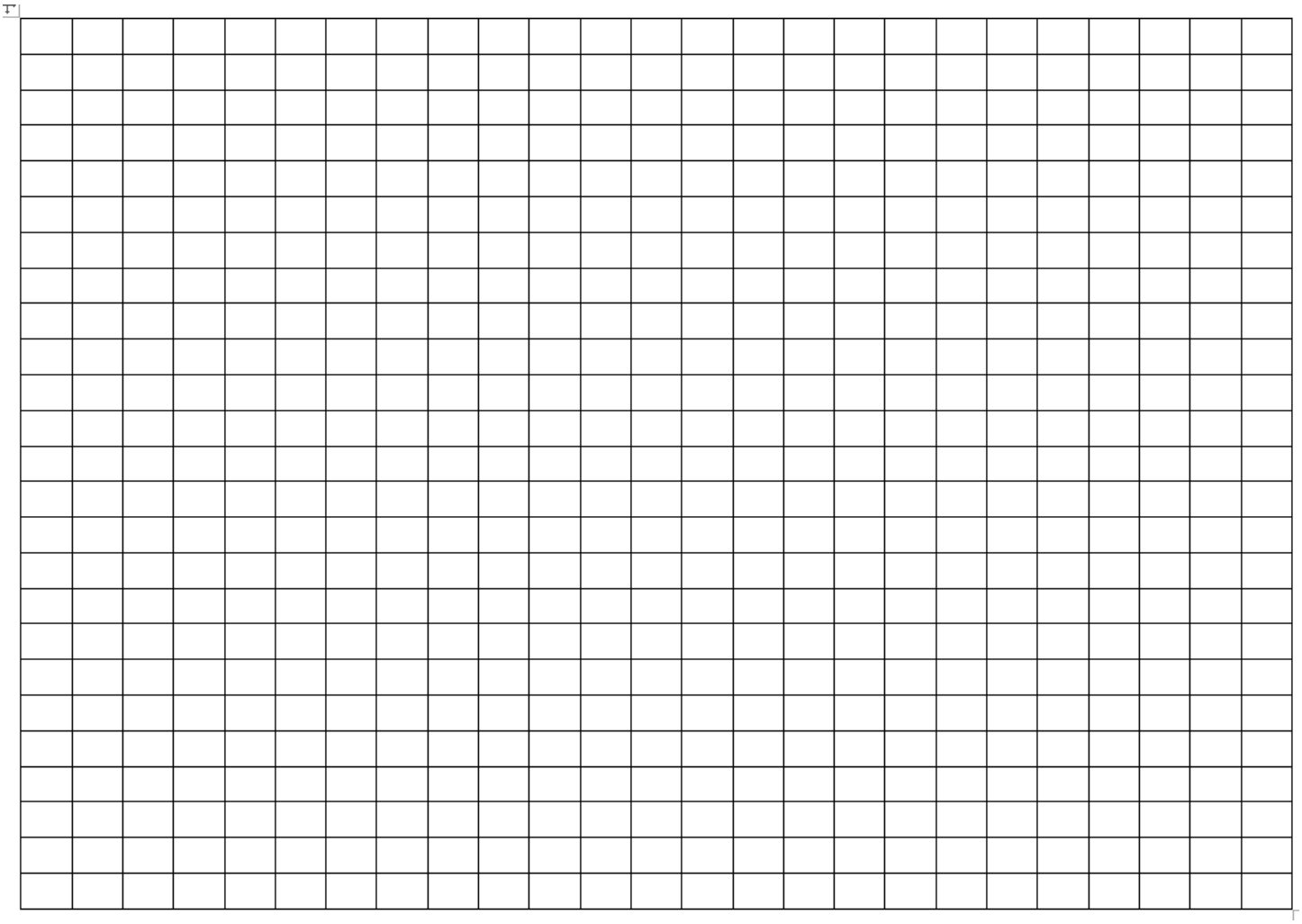
Part 3: Design Your Own Experiment

You will run three trials. Each one should have 100 total molecules**.** *Start with different amounts of A and B for each trial* (you cannot use the same amounts used earlier in this activity.) Place the starting amounts in the table at time 0. Record the amount of A and B in the chamber every 20 seconds for 5 minutes.

Trial 1			Trial 2			Trial 3		
Time	A	B	Time	A	B	Time	A	B
0 (initial)			0 (initial)			0 (initial)		
20			20			20		
40			40			40		
60			60			60		
80			80			80		
100			100			100		
120			120			120		
140			140			140		
160			160			160		
180			180			180		
200			200			200		
220			220			220		
240			240			240		
260			260			260		
280			280			280		
300			300			300		
Final A:B Ratio			Final A:B Ratio			Final A:B Ratio		

1. Which side of the reaction is favored (are there more reactants or products) for the experiment you set up? Why is that so?

2. Graph the concentration (number of molecules) of both molecules A and B vs time. You should have two separate curves (A and B). Remember, a good graph has a title, axis labels with units, and a key.



3. What is happening to the concentrations at the beginning of the experiment? How does that differ from what is happening at the end of the experiment? Mark a vertical line on the graph at the point where equilibrium is established.

4. All three trials started at different amounts. How did the final ratios of A to B compare?

5. Did the reaction ever stop? Why?