Instructions: Group Equilibrium PreLab

PART I: Go on-line and load the mc^2 Equilibrium Simulator:

http://mc2.cchem.berkeley.edu/Java/equilibriurn/

The simulator presents a dynamic, reversible process where two molecules of A (red spheres) collide with each other to form 1 molecule of B (blue sphere), which in turn breaks down and produces 2 molecules of A.

$$A + A \rightleftarrows B$$
$$2A \rightleftarrows B$$

Using the Equilibrium Simulator

The Equilibrium Simulator allows you to experiment with the variables relating to reaction rate, the extent of a chemical reaction, and equilibrium concentrations. It allows changes in the following parameters:

Red Probability (RP): A number between 0 and 1, where 1 represents the situation where *every* collision between two red particles results in the formation of a blue particle. If the RP were set to 0, *none* of the collisions between red particles would form a blue particle.

Blue Probability (BP): A number between 0 and 1, where 1 represents the situation where *every* collision a blue particle undergoes (with either the wall or another red or blue particle) results in the formation of two red particles. If the BP were set to 0, *none* of the collisions of blue particles would form red particles.

Red Number: Allows you to change the number of red particles: a number between 0 and 39.

Blue Number: Allows you to change the number of blue particles: a number between 0 and 39.

Temperature: Allows you to change the temperature and thus the speed of the particles. Higher temperatures mean faster speeds and more collisions between particles.

After entering the desired parameters click on **Equilibrate!**, which starts the "reaction." Click on **Pause** to stop the reaction. For best performance, turn all other software applications off.

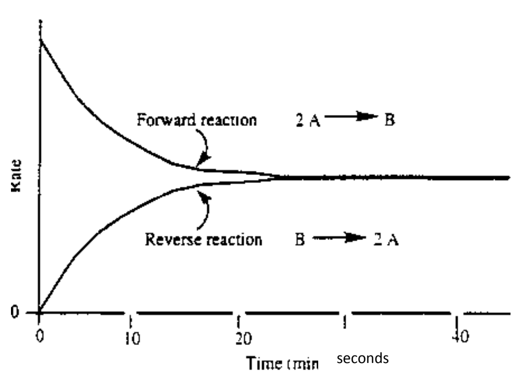
Questions and instructions:

1. a. Enter the following parameters, have a timer or watch available, and click on **Equilibrate (lower right button)** to start the reaction. Record the respective number of red and blue spheres at 5 sec., 10 sec., 15 sec., 20 sec. and 3 min.

Red Number	20	Red Probability	0.1
Blue Number	0	Blue Probability	0.1
Temperature	273		

b. At the instant the reaction begins, what is the rate of the reverse reaction, that of **B** going to **A**? Explain in the context of a microscopic view of the collisions of molecules.

Refer to the following graph: rates of the forward and *reverse reactions* vs. time starting with only A.



c. How does the rate of change in A compare to B from 0 to 10 sec? 1) increases 2) equals 3) decreases
d. How does the rate of change in A compare to B from 1 to 3 minutes? 1) increases 2) equals 3) decreases

True/False

At time = 0 seconds:

e. The rate of the forward reaction exceeds the rate of the reverse reaction.
f. The rate of the reverse reaction exceeds the rate of the forward reaction.
g. For a period of ~20 sec. after initial mixing, the concentration of the products increases.
h. For a period of ~20 sec after initial mixing, the concentration of the reactants increases.

At equilibrium:

i. The rate of the forward reaction is zero.
j. The rate of the reverse reaction is zero.
k. The rate of the forward reaction is equal to the rate of the reverse reaction.
l. The rates of the forward and reverse reactions are both constant.

2. Write the equilibrium expression for the reaction.

Using the equilibrium concentrations in question #1 calculate Kc.

3. Reset the simulator. Enter the following parameters and click on **Equilibrate (lower right button)** to start the reaction.

Red Number	15	Red Probability	1
Blue Number	5	Blue Probability	1
Temperature	273		

Record the respective number of red and blue spheres at 3 min.
Calculate Kc.

4. Reset the simulator. Enter the following parameters and click on **Equilibrate (lower right button)** to start the reaction.

Red Number	5	Red Probability	1
Blue Number	15	Blue Probability	1
Temperature	273		

Record the respective number of red and blue spheres at 3 min.
Calculate Kc.

5. Compare the calculated values of Kc for the three trials. What is their average and average deviation? What do you conclude about different starting concentrations and Kc.

PART II: Go on-line and load Dr. Nutt's / Davidson College's Equilibrium Simulator:

http://www.chm.davidson.edu/ronutt/che115/equkin/equkin.htm

This simulator presents the same dynamic, reversible process as in Part I.

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1. Select 80 molecules of **A** and a temperature of 298 **K**. Click the "On" button and observe the animation for ***three minutes***. Record the values of Red spheres, Blue spheres, and K_c at ***three minutes***.
2. Select 80 molecules of **A** and a temperature of 380 **K**. Click the "On" button and observe the animation for ***three minutes***. Record the values of Red spheres, Blue spheres, and K_c at ***three minutes***. In what way are the plots in the two questions (#1 and #2) similar, how do they differ?
3. Is this reaction exothermic or endothermic. Briefly explain the reasons for your selection.

Answer all questions on the prelab form. Be sure that the names of all Group members are included.