In-class assignment 3 - Kinetics Workshop

Names and roles: Manager: ___________________________

Recorder:___________________________

Presenter:___________________________

Technician:____________________________

Instructions: This exercise is designed to help you understand reaction kinetics. It will be done by making use of the simulator (CheerpJ version) found at the following link:

http://phet.colorado.edu/en/simulation/reactions-and-rates

To ensure that your team functions well in this workshop, you will each have a specific role. The roles are as follows:

Manager

Manages the group. Ensures that members are fulfilling their roles, that the assigned tasks are being accomplished on time, and that all members of the group participate in activities and understand the concepts. They are also responsible for answering questions from the teacher during class discussions.

Recorder

Records the names and roles of the group members at the beginning of each activity. Records the important aspects of group discussions, observations, insights, etc. The recorder's report is a log of the important concepts that the group has learned. They are also responsible for handing in the group's copy of the exercise.

Presenter

This person is responsible for reading each of the steps in the exercise to the group. They are also responsible for finding resources to help the group with their task.

Technician

Gathers materials. Performs all technical operations for the group, including the use of a calculator or computer.

Part 1 – Energy of collision

This exercise is an investigation into a) the factors that affect how reactants become converted into products and b) what factors may hinder the ability of a reaction to occur. This will be discussed in the context of *collision theory*, which suggests that a chemical process *can* take place when two or more reactants collide in space but it is not a guarantee. If the collision occurs under the right conditions, the bonds between the reactants can break and the products can then be formed.

We will begin by observing a hypothetical reaction: A + BC → AB + C. The atom, A, is represented by a yellow sphere and the molecule BC is composed of both a purple and blue sphere.

Step 1) Click on the green "+ sign" in the box marked "Separation View". The purpose of this window is to track how far apart your reactants are at different times of the reaction.

Step 2) Click on the green "+ sign" button in "Energy View". This should reveal a reaction coordinate diagram.

Q1) What does a reaction coordinate diagram describe?

Q2) What do the y and x-axis represent?

Q3) What does the difference (on the y-axis) between the apex of this curve and the initial reactant energy represent?

Q4) Is this reaction exothermic or endothermic? What feature suggests this?

Q5) How would you determine ΔH for this reaction?

Step 3) Pull the plunger *one-third* of the way down and release it. Click the "Pause" button after the reactants have collided *once*.

Q6) What happened?

Q7) What does the green "Total Energy" bar appearing in the reaction coordinate diagram represent? How is it related to how far you drew back the plunger?

Q8) What do you think the minimum position of the Total Energy bar has to be on the Y-axis for this reaction A + BC $\rightarrow$ AB + C to occur?

Step 4) Click on the "Reload Launcher" button. Pull back the plunger so that the Y-axis position of the green Total Energy Line is that which you suggested in Q8. Release the plunger and "Pause" after one collision.

Q9) Did it work? If not, try this again by changing the Y-axis position of the Total Energy line.

Q10) What can be concluded about the energy required for a reaction to occur?

Step 5) Reload the launcher and launch the particle at full energy, but this time allow the simulation to continue for ~1 min. Repeat as necessary to answer the following:

Q11) What happens when <u>the products,</u> AB + C collide?

Q12) Refer to your reaction coordinate diagram. Explain from an energy standpoint why the products can reconvert back into reactants?

<u>Part 2 – Effective collisions</u>

Step 1) Reload the launcher and click on "Angled Shot". Rotate the plunger all the way to the left and fire the particle with full energy. Observe the eventual collision. Re-test at several different angles.

Q1) In your simulations did the reaction have enough energy to occur?

Q2) Based on the angled shot simulation, does the angle at which the collision takes place play a vital role in the reactants becoming products? Explain.

Part 3 – Effect of temperature

Step 1) Click on "Reset All". Perform the reaction again at full energy, but slowly cool the reaction by dragging the bar below zero in the "Temperature" box. Stop cooling when the "Total Energy" line lies below the activation energy.

Q1) What role does temperature play in the likelihood of a reaction occurring?

Q2) Continue to cool the reaction. What happens to the speed of the particles when you cool the container?

Q3) In what way does temperature play a role in a collision being effective? What property of the collision does temperature affect, the angle of the collision or the kinetic energy of the colliding particles?

Part 4 – Effect of molarity

Step 1) Click on the "Many Collisions" tab.

Step 2) Click on the "Pause" button, then click on the "Show Stopwatch" option. Press "Start" on the Stopwatch

Step 3) Add 3 atoms of "A" and 3 molecules of "BC".

Step 4) Press "Play" and immediately heat the reaction so that the "Total Average Energy" bar in the Reaction Coordinate Diagram is half the activation energy. Observe the reaction until the stopwatch reads 500. Press "Pause".

Q1) What happened?

Q2) Do all the A atoms move at the same speed? What does that mean about their individual kinetic energies?

Q3) What about all the remaining particles? Do they move at the same speed?

Q4) Given your answers to Q2 and Q3, what does the "Total Average Energy" represent in the Many Collisions simulation?

Step 5) Press "Reset All" then add 15 particles of both A and BC. Press "Play", heat the system to half the activation energy and observe until the stopwatch reads 1500 time units. Repeat this step as necessary to answer the following questions.

Q5) What effect did increasing the molarities of A and BC have on the rate of formation of product?

Q6) What happened to the # of collisions observed as you increased the # of reactants?

Q7) How might losing reactants over time slow down the rate of the reaction?

Q8) How might producing more product over time hinder the rate the reaction (look closely at what the products do in the simulation)?

Part 5 – Multiple reactants (molecularity)

Imagine the following scenarios:

a) You are meeting one friend at the mall but haven't agreed on where. When you get there, the cell phones of both you and your friend die. You start walking randomly to meet each other.
b) Same scenario as in (a) but there are three of you that had agreed to meet up.

Q1) In which scenario is it more likely that *you and all of your friends* will meet randomly at *exactly the same place* and at *exactly the same time*? Why?

Now consider the following hypothetical reaction: A + B + CD → ABCD

You test this reaction in the lab and note that the products form at a far slower rate than the reaction you studied in the previous simulations, i.e. A + BC → AB + C

Q2) How many reactants (atoms or molecules) are involved in the chemical equation A + BC→ AB + C? Q3) How many reactants (atoms or molecules) are involved in the chemical equation A + B + C → ABC? Q4) The reaction in Q3 is slower than that in Q2. How does the # of reactant atoms/molecules in a chemical equation (what is known as *molecularity*) affect reaction speed? Consider this in the context of effective collisions and take inspiration from the mall scenarios answered earlier.

Q4) The reaction A + B + CD → ABCD is even slower than the reaction in Q3 despite having similar activation energy and a similar molecularity (HINT: Think back to another criteria for an effective collision to occur)?

Summary

Briefly summarize how each of the following factors influences the rate of a reaction:

1) The activation energy:

2) An orientation of the collision:

3) The temperature of the reaction:

4) The molarity of the reactants:

5) The number of reactants involved in the collision (molecularity):