In-class assignment 3 - Kinetics Workshop Answer Key

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?

It describes the energetics involved in reactants becoming products. Represented are the activation energy of the reaction and the overall enthalpy change.

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

Energy and reaction coordinate.

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

The activation energy.

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

Endothermic as the energy of the products is more than those of the reactants.

Q5) How would you determine ΔH for this reaction?

The difference in energy between the products and reactants.

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?

A collided into BC but no reaction occurred.

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?

The total energy available to the system.

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 → AB + C to occur?

Above the activation energy.

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?

For a reaction to occur, the kinetic energy available to the reactants must be more than the activation energy.

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 the products, AB + C collide?

They converted back into the reactants.

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

There is sufficient energy in the system for the products to overcome the reverse activation energy.

Part 2 – Effective collisions

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?

Yes

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.

For a reaction to be effective, you not only require enough energy but the angle of the collision (orientation) has an impact as well.

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?

It determines how much kinetic energy the reactant particles have.

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

They slow down.

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?

When the temperature is higher, the particles have more energy available and collisions can be more effective. When cooler, the lack of energy available reduces the likelihood of an effective collision.

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?

Although many collisions occurred, not all were successful at making product.

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

No, they all have different KE.

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

Same as atom A.

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

The average energy (KE) associated with all the particles in the system.

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?

It increased the number of successful collisions (it should).

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

There were more as more particles were present in the reaction space.

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

It reduces the likelihood of reactants finding each other so effective collisions become less frequent.

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

These products can also successfully collide to form back reactants or they may even impede reactants from finding each other to make successful collisions.

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?

The first as the probability of two people meeting at the same time is better than three.

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?

Two

Q3) How many reactants (atoms or molecules) are involved in the chemical equation A + B + C → ABC?

Three

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.

Yes, it does. It is harder for reactants in Q3 to successfully collide at the same time and with the correct alignment. This leads to rarer effective collisions which reduces the speed.

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)?

The CD molecule likely requires an additional orientation factor.

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):