Dry Lab 2: Understanding the Equilibrium Condition

The task of your group is to investigate the equilibrium of the reaction

$$A(g) \leftrightarrows B(g)$$

Information about the reaction you are studying:

1) It is known that, kinetically, the reaction is **first order** in A for the forward direction and in B for the reverse direction.
2) At 25°C, the rate constant, k_f, for the forward reaction is 0.10 s^{-1}. At this temperature, the rate constant for the reverse reaction, k_r, is 0.25 s^{-1}
3) At 60°C, the rate constant, k_f, for the forward reaction is 0.50 s^{-1}. At this temperature, the rate constant for the reverse reaction, k_r, is 0.30 s^{-1}.

Based on the information above, write the *rate law expression* for the forward reaction and the reverse reaction in the space below at 25°C

Rate$_f$ =
Rate$_r$ =

Answer the following questions.

a) How will the rate law expressions **change** if they were rewritten for 60°C as opposed to 25°C ? Explain.
b) Does it make sense that the k values for the reactions increased between 25°C and 60°C? Explain on a molecular level why.

Reactions to Investigate:

Group A)

1) You are given a mixture that is at 25°C. The initial concentration of A, $[A]_0$, is 5.00 M. There is no B initially. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.
2) You are given a mixture that is at 60°C. The initial concentration of A, $[A]_0$, is 5.00 M. The initial concentration of B, $[B]_0$ is also 5.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.

Group B)

1) You are given a mixture that is at 25°C. The initial concentration of A, $[A]_0$, is 10.00 M. There is no B initially. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.
2) You are given a mixture that is at 60°C. The initial concentration of A, $[A]_0$, is 4.00 M. The initial concentration of B, $[B]_0$ is 5.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.

Group C)

1) You are given a mixture that is at 25°C. The initial concentration of A, $[A]_0$, is 2.00 M. The initial concentration of B, $[B]_0$, is 6.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.
2) You are given a mixture that is at 60°C. The initial concentration of A, $[A]_0$, is 0.00 M. The initial concentration of B, $[B]_0$ is 8.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.

Group D)

1) You are given a mixture that is at 25°C. The initial concentration of A, $[A]_0$, is 0.00 M. The initial concentration of B, $[B]_0$, is 5.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.
2) You are given a mixture that is at 60°C. The initial concentration of A, $[A]_0$, is 4.00 M. The initial concentration of B, $[B]_0$, is also 6.00 M. Please determine when this system reaches equilibrium and the concentrations of [A] and [B] at that time. Use the table and graph paper on the next pages to guide you.

Scenario 1 (25°C)

Time (s)	**[A]**	**△A/△t**	**[B]**	**△B/△t**
0				
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21				
22				
23				
24				
25				

Has your system reached equilibrium by 25 seconds? How do you know? Clearly graph the concentrations of [A] and [B] as a function of time.

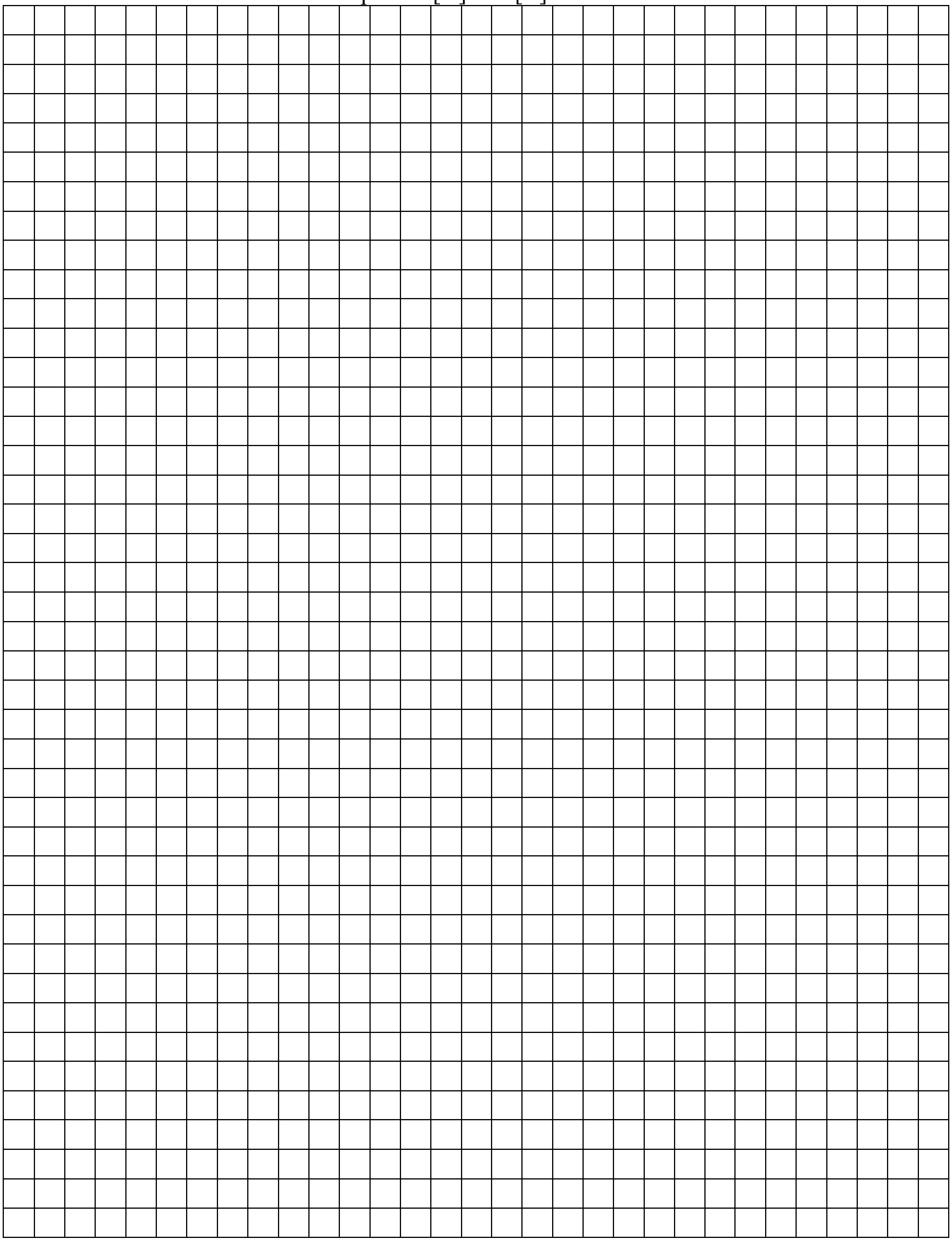
Scenario 2 (60°C)

Time (s)	[A]	△A/△t	[B]	△B/△t
0				
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21				
22				
23				
24				
25				

Has your system reached equilibrium by 25 seconds? How do you know? Clearly graph the concentrations of [A] and [B] as a function of time.

Graph I – [A] and [B] at 25^o**C**

Graph II – [A] and [B] at 60^{o}**C**



Follow Up Equilibrium Assignment

Methanol, $CH_3OH(g)$, can be synthesized from the reaction of carbon monoxide gas and hydrogen gas, as shown by the balanced chemical equation below:

$$CO(g) + 2H_2(g) \leftrightarrows CH_3OH(g)$$

A student initiates a study by performing two experiments at 27°C. In the first experiment, the student mixes 1.000 M CO(g) with 3.000 M $H_2(g)$ and monitors the [CO] as a function of time. Results of this are shown below:

Time (min)	**[CO]**	**[H_2]**	**[CH_3OH]**
0	1.000	3.000	0
10	0.837		
20	0.764		
30	0.638		
40	0.592		
50	0.586		
60	0.586		

a) Based upon the data in the table, is it correct to say the reaction system has reached equilibrium? Justify your answer.
b) Determine the [H_2] and [CH_3OH] for all other times in the table.
c) Write the equilibrium constant expression for the reaction above and determine its value for this reaction

For the second experiment, the student uses only a pressure sensor. Into a 4.0 L container, the student places 0.406 moles of $CH_3OH(g)$. The reaction system is maintained at 27°C at all times. The student then monitors the **total** pressure of the system. Data on this is shown below:

Time(Min)	P_{tot} (atm)	P_{CO} (atm)	P_{H2} (atm)	P_{CH3OH} (atm)
0	2.500			
10	4.900			
20	6.630			
30	7.460			
40	7.470			

d) Verify the initial pressure in the container should be 2.50 atm
e) What is the value of the initial reaction quotient, Q for this system?
f) Explain conceptually why the pressure must **increase** as the reaction proceeds
g) Is it fair to say this system has reached equilibrium? Justify your answer.
h) Determine the partial pressures of each gas in the container and add those to the appropriate cells above
i) What is the equilibrium constant for this process? Justify your answer
j) Are the equilibrium constants the same for both experiments? Should they be? Justify your answer.

k) Determine the value of the equilibrium constant (Kp and Kc) at 27°C for each of the following reactions:

I) $2CO(g) + 4H_2(g) \leftrightarrows 2CH_3OH(g)$
II) $CH_3OH(g) \leftrightarrows CO(g) + 2H_2(g)$
III) $10CH_3OH(g) \leftrightarrows 10CO(g) + 20H_2(g)$

The same student studies two additional systems of $CO(g)$, $H_2(g)$, and $CH_3OH(g)$ at 27^oC

System	**[CO]**	**[H_2]**	**[CH_3OH]**
3	0.788	0.975	0.112
4	2	2	2

l) Is either system initially in equilibrium? Justify your answer
m) For any system(s) **NOT** in equilibrium, determine the equilibrium concentrations of the reactants and products.

Dry Lab 2: Understanding the Equilibrium Condition

(Teacher Notes)

Prerequisite Concepts:

- Understanding the Equilibrium Condition
- Ability to write rate laws and utilize rate expressions

Introduction for Teachers:

The purpose of this assignment is to allow students to understand the nature of the amounts of reactants and products under various conditions. Students should already have an understanding of what is happening conceptually in terms of rates when the equilibrium condition is reached. This assignment motivates the *Law of Mass Action*, getting students to understand that a function of the concentrations of the reactants and products determines the equilibrium state. Each reaction studied is an elementary reaction from kinetics, and in these situations, it is possible to quickly determine the equilibrium state by calculating how the reactants and products change over time according to the rate laws written. Students then graph the data and discover that the ratio of the reactants to products is always fixed at a given temperature independent of the initial concentrations.

Students should get that the rate law for each reaction is:

$Rate_f = k_f[A]$

$Rate_r = k_r[B]$

Of course these expressions will not change for the higher temperature save for the larger value of k, which makes sense on a molecular level as there will be more collisions with sufficient correct orientation and energy to overcome the activation energy barrier.

It is critical to note that this setup is special in the sense that kinetics and thermodynamics are separate fields, and *only in the case of reactions that occur in a single elementary step* can equilibrium constants be determined in the way shown in this Dry Lab. What we wish to motivate here is that K depends on a ratio of products to reactants and is only temperature dependent. Extra work will need to be done in class to discuss how to extend the Law of Mass Action to generic reactions (including heterogeneous systems) and to look at the difference between K_p and K_c. A follow-up assignment is attached that will allow you to test student understanding after these topics have been covered.

In this dry lab, you might consider splitting your class into 4 groups and have each investigate one system at each temperature. Although only 4 situations are given, it is simple to add other scenarios as the initial concentrations of A and B are only limited by your imagination. However, it is important that at least one group start with all A, one with all B, and one with a 50-50 mixture of the two as the last in particular is a situation that most student believe is an equilibrium condition. When the groups are done and certain their system is in equilibrium, you might have each report their value of [A] and [B] and then together calculate the ratios. Students are surprised to see that the ratio stays fixed in all scenarios for a given temperature.

You will find an excel spreadsheet on the CD that is set up to calculate the graphs for [A] and [B] under various conditions. In addition, the answers to the follow up assignment are on sheet 2.

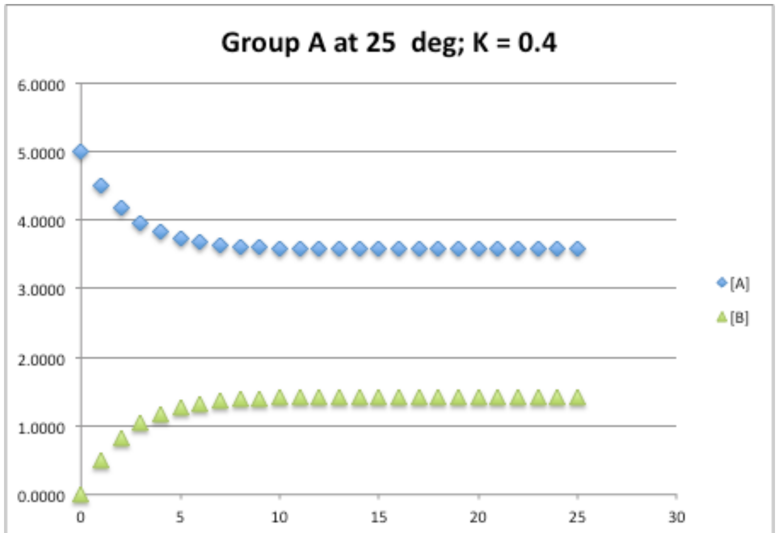
Common Student Errors:

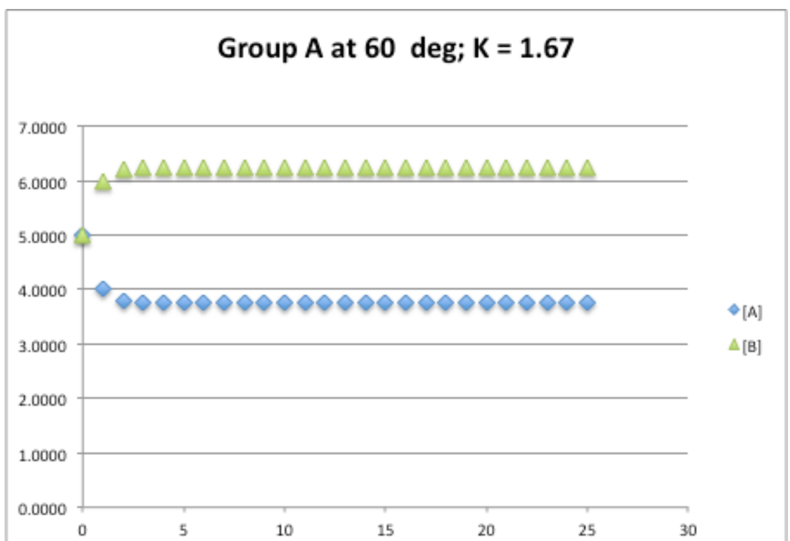
Make sure that students understand how to write both the rate expression and understand how to calculate the concentrations of A and B at each step as the reaction approaches equilibrium. Students will not understand that the $[A]_i = [A]_{i-1} - d[A]/dt + d[B]/dt$ and $[B]_i = [B]_{i-1} - d[B]/dt + d[A]/dt$. It is good to walk around from group to group and check that one step has been done correctly.

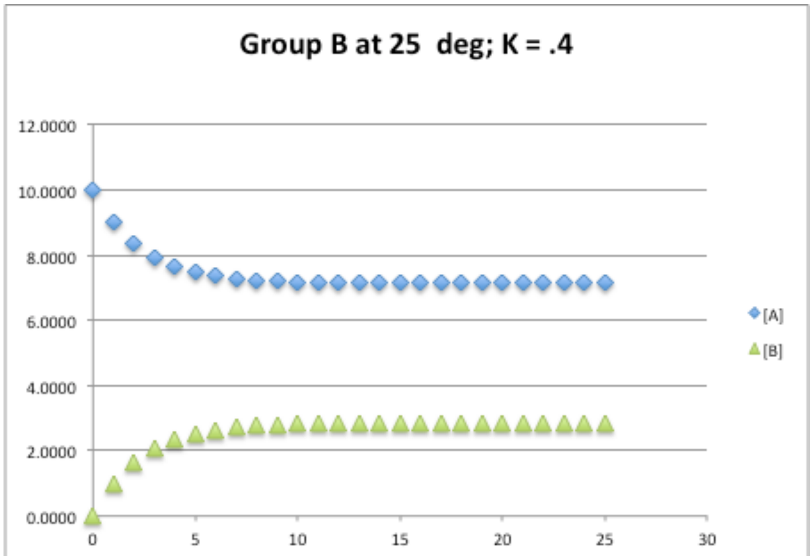
Graphs of each scenario (can be recreated in attached Excel spreadsheet)

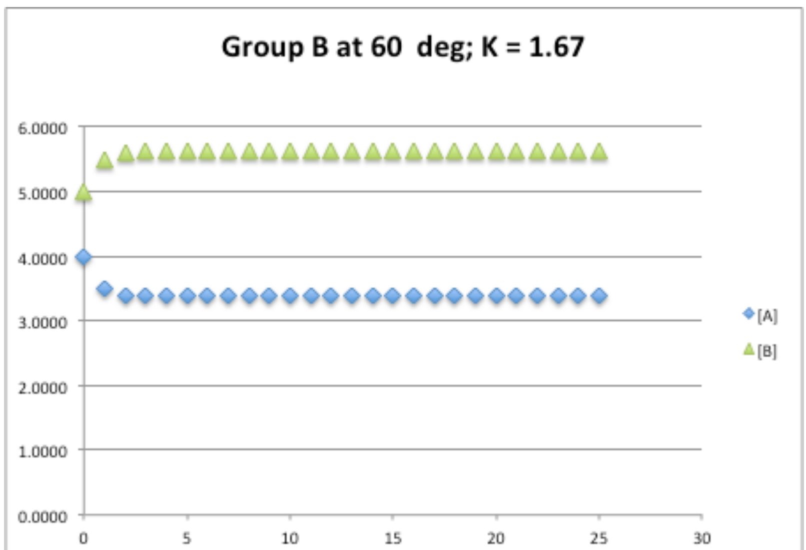
Note for each graph at 25^{o}C: k_f = 0.10 ; k_r = 0.25

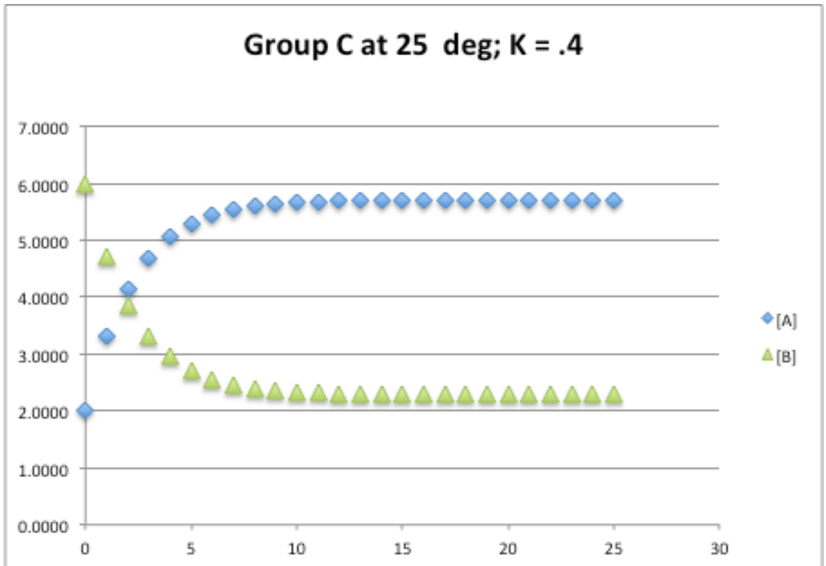
Note for each graph at 60^{o}C: k_f = 0.50 ; k_r = 0.30

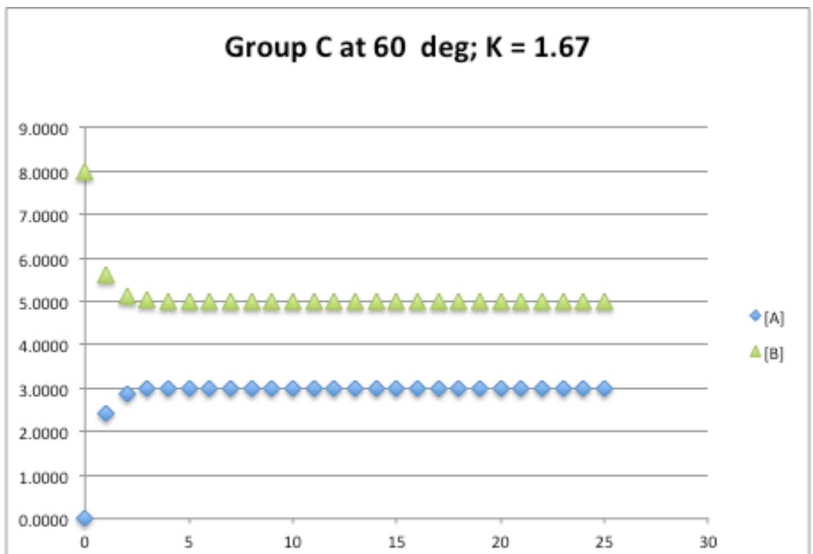


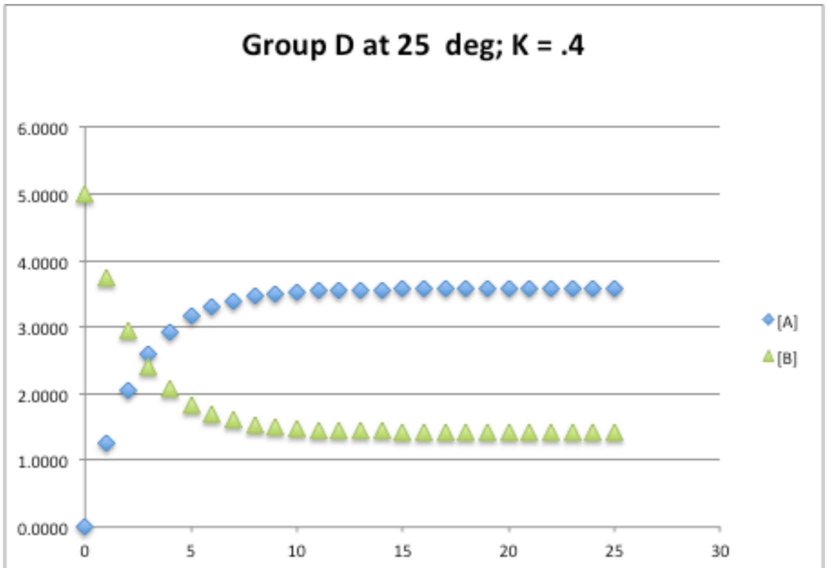


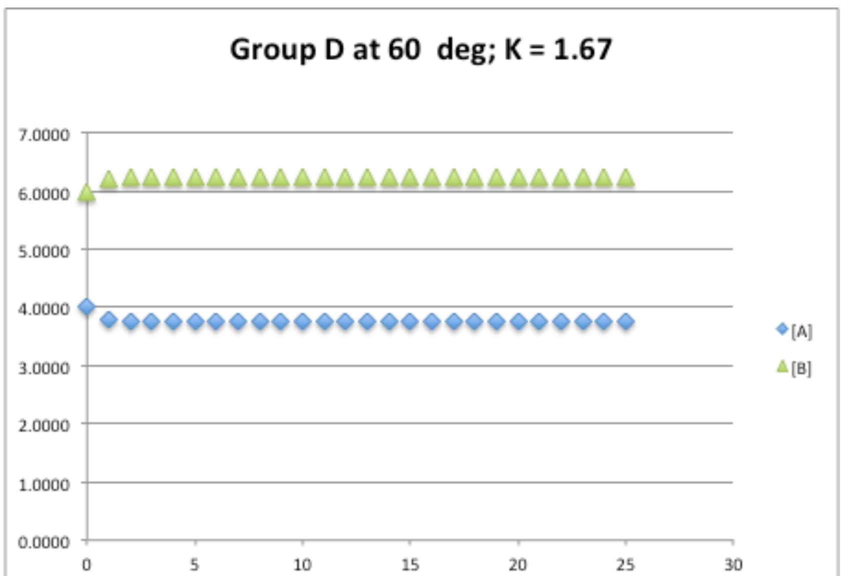

Group B at 25 deg; K = .4
12.0000
10.0000
8.0000
6.0000
4.0000
2.0000
0.0000
0
5
10
15
20
25
30
[A]
[B]


Group B at 60 deg; K = 1.67
6.0000
5.0000
4.0000
3.0000
2.0000
1.0000
0.0000
0
5
10
15
20
25
30
[A]
[B]


Group C at 25 deg; K = .4
7.0000
6.0000
5.0000
4.0000
3.0000
2.0000
1.0000
0.0000
0
5
10
15
20
25
30
[A]
[B]


Group C at 60 deg; K = 1.67
9.0000
8.0000
7.0000
6.0000
5.0000
4.0000
3.0000
2.0000
1.0000
0.0000
0
5
10
15
20
25
30
[A]
[B]





Rubric: Understanding the Equilibrium Condition

10 pts – You seem to have complete understanding!

9 pts – Fairly forward thinking; there's no going back on your part!

8 pts – Why were we given different temperatures? K is always constant!?

7 pts – Hard to climb back up a slippery slope, isn't it!

6 pts – What are those graphs for anyway?