During Class Inventions and Computer Lab Activities



Volume II 3RD EDITION

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During Class Inventions*



Kinetics

Introduction to Kinetics Rates of Reaction Method of Initial Rates Integrated Rate Law Part I Half-Life Integrated Rate Law Part II Temperature Dependence of the Rate Constant Reaction Mechanisms

Equilibrium

Extent of a Reaction Calculating the Equilibrium Constant for a Reaction Calculating the Equilibrium Concentration of all Species Le Châtelier's Principle Non-Equilibrium Reaction Quotient Temperature Dependence of the Equilibrium Constant

Acids and Bases

Arrhenius Acids, [H*], [OH-], pH and pOH
Brønsted-Lowry Acid/Base Theory Acids, Bases and pH
Strong Acids and the Equilibrium Constant
Weak Acids and the Equilibrium Constant
Polyprotic Acids
Salts I
Salts I

Aqueous Equilibrium:

The Common Ion Effect Neutralization Reactions Titration Between a Strong Acid and a Strong Base Titration Between a Weak Acid and a Strong Base Introduction to Buffers Buffers Precipitation and Solubility Solubility Equilibria Problems

Thermodynamics

Enthalpy and the First Law Spontaneity and Entropy Spontaneity and Free Energy Free Energy and Equilibrium Constant

Electrochemistry

Introduction to Oxidation Reduction Galvanic Cells EMF for Galvanic Cells Nernst Equation Batteries Electrolysis I Electrolysis II

* The bulk of the activities in this section were originally developed and tested by John Gelder. Some of the activities were developed by Michael Abraham. Others were developed and tested by Thomas Greenbowe, Marilyn Stains, and Nihal Kaissieh at the University of Arizona and Iowa State University.

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INTRODUCTION TO KINETICS

Name

Section

1. List four factors that affect the rate of a chemical reaction. For each, provide a brief statement describing how it affects the speed of a chemical reaction.

- 2. a. Define the term *reaction rate*.
 - b. For the following chemical reaction

$$2N_2O_5(g) \rightarrow 4NO_2(g) + O_2(g)$$

write a rate expression in terms of

- i. the change in concentration of $\mathrm{N_2O_5}$ with time;
- ii. the change in concentration of NO_2 with time;
- iii. the change in concentration of O_2 with time;

- iv. write a statement that compares the rate of appearance of NO_2 to the rate of appearance of $\mathrm{O}_2;$
- v. write a mathematical equation that equates the rates of the reactants and products in the reaction to each other.
- 3. In the plot below, three lines, labeled A, B, and C are shown. Identify (use the letter) which line best represents the *average rate*, *instantaneous rate* and *initial rate* for the chemical reaction.



RATES OF REACTION

Name

Section

1. a. Given the following data

Time (min)	Exp. #1 [NO ₂] (M)	Exp. #2 [NO ₂] (M)
0	0.350	1.05
2	0.289	0.583
4	0.245	0.324
8	0.190	0.0999
16	0.130	0.0095
24	0.090	0.0009
40	0.062	

for the reaction $2NO_2(g) \rightarrow 2NO(g) + O_2(g)$

The data for Exp. #1 is plotted below. Determine the average rate of the reaction between 8 and 24 min., the instantaneous rate of the reaction at 8 minutes and the initial rate of the reaction.



b. The data for Exp. #2 is plotted below. Determine the average rate of the reaction between 8 and 24 minutes, the instantaneous rate of the reaction at 8 minutes and the initial rate of the reaction.



- c. By what factor did the initial concentration change in going from Exp. #1 to Exp. #2?
- d. By what factor did the initial rate change in going from Exp. #1 to Exp. #2?
- e. Write an equation which describes how the initial rate of the reaction depends on the initial concentration.

METHOD OF INITIAL RATES

Name

Section

- 1. Define the terms *rate expression* and *rate law* for a chemical reaction.
- 2. Write the general rate law for the following reaction

$$2NO(g) + Cl_2(g) \rightarrow 2NOCl(g)$$

Identify the rate constant in the rate law. What are the exponents in the rate law called?

3. What experimental data is needed to determine the order of a chemical reaction?

4. a. Consider the reaction

$$2\mathrm{NO}(g)+2\mathrm{H_2}(g)\to\mathrm{N_2}(g)+2\mathrm{H_2O}(g)$$

and the following initial rate data.

Experiment Number	P _{NO} (mmHg)	P _{H2} (mmHg)	Initial Rate $\left(\frac{mmHg}{s}\right)$
1	400	150	0.66
2	400	300	1.34
3	150	400	0.25
4	300	400	1.03

i. Determine the reaction order for NO and H_2 .

ii. Determine the overall order of the reaction.

iii. Write the specific rate law for the reaction.

iv. Determine the rate constant for the reaction (include units).

b. The following initial rate data were collected for the reaction at 100 °C.

$$2\mathrm{NO}_2(g) + \mathrm{F}_2(g) \to 2\mathrm{NO}_2\mathrm{F}(g)$$

Exp.	[NO ₂]	[F ₂]	initial rate (M/sec)							
1	0.0482 M	0.0318 M	1.90×10^{-3}							
2	0.0120 M	0.0315 M	4.69×10^{-4}							
3	0.0480 M	0.127 M	$7.57 imes 10^{-3}$							

i. Determine the reaction order for NO_2 and F_2 .

ii. Determine the overall order of the reaction.

iii. Write the specific rate law for the reaction.

INTEGRATED RATE LAW PART I

Name

Section

1. The reaction: $A(g) \rightarrow$ products

follows simple first order kinetics. When the initial concentration of A is 0.500 M, the initial rate of the reaction is determined to be $4.20 \times 10^{-3} \text{ M s}^{-1}$. If the initial concentration of A is tripled, what would be the new initial rate of the reaction?

2. Write the integrated rate law for a reaction that follows simple first order kinetics.

3. The decomposition of H_2O_2 to H_2O follows first order kinetics with a rate constant of 0.0410 min⁻¹ at a particular temperature.

$$\mathrm{H_2O_2}(l) \ \rightarrow \ 2\mathrm{H_2O}(l) \ + \ \mathrm{O_2}(g)$$

Calculate the $[H_2O_2]$ after 10 minutes, if $[H_2O_2]_0$ is 0.200 M.

4. The decomposition of N₂O₅ to O₂ and NO₂ follows first order kinetics. If a sample at 25 °C with the initial concentration of N₂O₅ of 1.25×10^{-3} M falls to 1.02×10^{-3} M in 100 minutes, calculate the rate constant for the reaction.

5. Describe how a plot of ln [concentration] versus time can provide the rate constant for a reaction that follows simple first order kinetics.

6. Using the following data, establish that the decomposition N_2O_5 according to the reaction,

$$2N_2O_5(g) \rightarrow 2NO_2(g) + O_2(g)$$

follows first order kinetics. Determine the rate constant for the reaction.

Time (sec)	[N ₂ O ₅] (M)
0	1.50×10^{-3}
2000	1.40×10^{-3}
5000	1.27×10^{-3}
7000	1.18×10^{-3}
11000	1.03×10^{-3}
15000	9.00×10^{-4}

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HALF-LIFE

Name

Section

1. a. For the reaction:

 $A(g) \rightarrow \text{products}$

when the $[A]_0 = 0.400 \text{ M}$, what will the concentration of A be after one half-life?

b. What additional information would you need to determine the concentration of the products in the reaction after one half-life?

2. Beginning with the general form of the integrated rate law for a reaction that follows simple first order kinetics, derive the mathematical equation for the half-life of the reaction.

3. The decomposition of H_2O_2 to H_2O and O_2 follows first order kinetics with a rate constant of 0.0410 min⁻¹ at a particular temperature.

$$\mathrm{H_2O_2}(l) \to 2\mathrm{H_2O}(l) + \mathrm{O_2}(g)$$

How long would it take for half of the $\mathrm{H_2O_2}$ to decompose?

INTEGRATED RATE LAW PART II

Name

Section

1. The reaction:

 $B(g) \rightarrow products$

follows simple second order kinetics. When the initial concentration of B is 0.500 M, the initial rate of the reaction is determined to be $8.40 \times 10^{-3} \text{ M s}^{-1}$. When the initial concentration of B is tripled, what change would you expect to observe in the initial rate of the reaction?

2. Write the integrated rate law for a reaction that follows simple second order kinetics.

3. a. The decomposition of NOCl(g)

 $2NOCl(g) \rightarrow 2NO(g) + Cl_2(g)$

is a second order reaction with a rate constant of 0.0480 $M^{-1} \cdot \sec^{-1}$ at 200 °C. In an experiment at 200 °C, the initial concentration of NOCl was 0.400 M. What is the concentration of NOCl after 15.0 minutes have elapsed?

- b. How many minutes will it take for the concentration of NOCl(g) to drop to 0.150 M?
- 4. Derive a mathematical equation for the half-life for a reaction which follows simple second order kinetics.

5. The initial concentration of NOCl, described in 3.a. above, is 0.400 M. Calculate the half-life for the decomposition reaction.

6. Describe how a plot of *ln* [concentration] versus time can provide the rate constant for a reaction which follows simple second order kinetics.

7. Using the following data, establish that the decomposition of NO_2 according to the reaction,

$$2NO_{2}(g) \rightarrow 2NO(g) + O_{2}(g)$$

follows second order kinetics. Determine the rate constant for the reaction.

Time (sec)	[NO ₂] (M)
0	0.0100
25	0.0088
50	0.0079
75	0.0071
100	0.0065
150	0.0055
175	0.0051
200	0.0048
250	0.0042
300	0.0038



TEMPERATURE DEPENDENCE OF THE RATE CONSTANT

Name

Section

1. a. The following rate data was obtained at different temperatures for the reaction

 $\mathrm{O_3}(g) + \mathrm{NO}(g) \to \mathrm{O_2}(g) + \mathrm{NO_2}(g)$

Temperature (K)	1/ _T	k (M⁻¹·sec⁻¹)	ln k
600		0.28	
650		0.22	
700		1.30	
750		6.00	
800		23.0	

Sketch the plot of ln k (y-axis) versus $\frac{1}{\text{temperature}}$ (x-axis)



b. Write the Arrhenius equation and identify each term.

c. Define the term *activation energy*.

- d. Determine the activation energy using the plot you made in 1a.
- 2. a. At 300 °C the rate constant for the reaction

$$\overset{\mathsf{CH}_2}{\underset{\mathsf{CH}_2}{\longrightarrow}} \overset{\mathsf{CH}_2}{\underset{\mathsf{CH}_2}{\longrightarrow}} H_2\mathsf{C}=\mathsf{CH}_2\mathsf{CH}_3$$

is 2.41×10^{-10} sec⁻¹. At 400 °C the rate constant is 1.16×10^{-6} sec⁻¹. Calculate the activation energy for the reaction.

b. Estimate the rate of the reaction at 800 °C.

c. If the activation energy for the decomposition of N_2O_5 is $1.0 \times 10^2 \frac{kJ}{mol}$, calculate the temperature change necessary to double the rate at room temperature.

3. Sketch the energy profile diagram for the exothermic reaction

$$NO(g) + O_3(g) \rightarrow NO_2(g) + O_2(g)$$

and label the important features, including reactants, products, activated complex, the energy of activation and the enthalpy of the reaction.

REACTION MECHANISMS

Name

Section

1. Given the chemical equation

$$R + BG \rightarrow RG + B$$

Describe the interaction between reactant particles that must occur to convert them to products. You may draw one or more pictures as part of your description.

2. Write the general differential form of the rate law for the reaction above.

3. The following table summarizes several experiments where the concentrations of R and BG were varied to determine the effect on the initial rate of the reaction.

Experiment Number	R (M)	BG (M)	Initial Rate (<u>M</u>)
1	0.240	0.125	$1.85 \ge 10^{1}$
2	0.480	0.124	3.68 x 10 ¹
3	0.479	0.249	7.37 x 10 ¹

Determine the rate law for the reaction.

4. How do the exponents in the rate law that was obtained in Question 3 compare to the coefficients in the balanced chemical equation in Question 1?

5. Define the term *reaction mechanism*.

6. a. Optional: Look at the simulation (http://introchem.chem.okstate.edu/DCICLA/K2GBM.htm) for the reaction:

 $2G + B \rightarrow G_2B$

The rate law is known to be rate = $k[G]^2$. Suggest a possible mechanism for this reaction.

b. Why is B not part of the rate law? (Hint: do all of the steps in a mechanism contribute to the overall rate? Why or why not?)

7. The rate law for the following reaction

$$2NO_2(g) + F_2(g) \rightarrow 2NO_2F(g)$$

was experimentally determined to be

rate =
$$k[NO_2]^1[F_2]^1$$

Which of the following mechanisms is the most reasonable? Explain your reasoning for making the choice you did.

a.
$$2NO_2(g) + F_2(g) \rightarrow 2NO_2F(g)$$

b.
$$\operatorname{NO}_2(g) + \operatorname{F}_2(g) \to \operatorname{NO}_2\operatorname{F}(g) + \operatorname{F}(g)$$
 (fast)
 $\operatorname{NO}_2(g) + \operatorname{F}(g) \to \operatorname{NO}_2\operatorname{F}(g)$ (slow)

c.
$$NO_2(g) + F_2(g) \rightarrow NO_2F(g) + F(g)$$
 (slow)
 $NO_2(g) + F(g) \rightarrow NO_2F(g)$ (fast)

8. Suggest a mechanism for the reaction

$$CH_3NC(g) \rightarrow CH_3CN(g)$$

if the experimental rate law is rate = $k[CH_3NC]^1$.

9. Suggest a possible mechanism for the reaction

$$OH^- + CH_2Br \rightarrow CH_2OH + Br^-$$

if the experimental rate law is rate = $k[CH_3Br]^1[OH^-]^1$.

10. Suggest a possible mechanism for the reaction

$$NO_{2}(g) + CO(g) \rightarrow NO(g) + CO_{2}(g)$$

if the experimental rate law is rate = $k[NO_2]^2$.

11. Consider the following set of equations

Step I:	$\operatorname{Cl}(g) + \operatorname{O}_3(g) \to \operatorname{ClO}(g) + \operatorname{O}_2(g)$
Step II:	$\operatorname{ClO}(g) \to \operatorname{Cl}(g) + \operatorname{O}(g)$
	$\mathrm{O_3}(g) \to \mathrm{O}(g) + \mathrm{O_2}(g)$

Describe the process illustrated by the above set of equations and the role each of the species plays in the process. Use words like mechanism, elementary steps, overall reaction, reactants, products, intermediate, and catalyst in your description.

EXTENT OF A REACTION

Name

Section

This DCI consists of a series of experiments that involve interaction between you (the student), your instructor and a molecular level simulation.[†] Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ERGBN.htm

 Open the Graphic Simulation program for the R + BG reaction. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table. Then determine the entries for the Concentration Change – C row.

EXPERIMENT #1:	R ·	+ BG ·	\rightarrow RG +	В
Initial Concentration – I	2.0	2.0	0	0
Concentration Change – C				
Ending Concentration – E				‡
e				

Notes, observations, and speculations:

⁺If you do not have access to this DCI's website link, your instructor will provide you with the data you will need to complete Experiments 1–5.

[‡]If you do not have access to the DCI website link, your instructor will provide the Ending Concentrations for RG and B.

2. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table. Then determine the entries for the Concentration Change – C row.

EXPERIMENT #2:	R +	BG –	→ RG +	В
Initial Concentration – I	1.0	1.0	0	0
Concentration Change – C				
Ending Concentration – E				†

Notes, observations, and speculations:

3. Predict the ending amount for these initial conditions

EXPERIMENT #3:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	1.5		1.5		0		0
Predicted							
Concentration Change – C							
Predicted							
Ending Concentration – E							

After making your predictions, adjust the initial conditions of the reaction being studied to those listed in the table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations below[†]. Then determine the entries for the Concentration Change.

Notes, observations, and speculations:

⁺ If you do not have access to the DCI website link, your instructor will provide the Ending Concentrations for RG and B.

4. Predict the ending amount for these initial conditions

EXPERIMENT #4:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	0		0		1.0		1.0
Predicted							
Concentration Change – C		_					
Predicted							
Ending Concentration – E		-		-			

After making your predictions, adjust the initial conditions of the reaction being studied to those listed in the table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations below[†]. Then determine the entries for the Concentration Change.

Notes, observations, and speculations:

5. Predict the ending amount for these initial conditions

EXPERIMENT #5:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	1.0		0.6		1.2		0.8
Concentration Change – C							
Ending Concentration – E							

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations below.[†] Then determine the entries for the Concentration Change.

Notes, observations, and speculations:

⁺ If you do not have access to the DCI website link, your instructor will provide the Ending Concentration for R.

6. Complete the following table

	R	+	BG	\rightarrow	RG	+	В			
Exp #1-Ending Conc –E		_								
Exp #2-Ending Conc –E										
Exp #3-Ending Conc –E		_						_		
Exp #4-Ending Conc –E		-						-		
Exp #5-Ending Conc –E		_						 _		

7. What conclusions can be drawn from these data? Find an algebraic equation that relates the ending concentrations of the reactants and products of the reactions being studied. (Hint: Try all possible combinations of the four concentrations by multiplication and/or division. For example, multiply all four concentrations together, multiply two and divide by the other two, etc., looking for the combination that gives the most constant result.) Summarize your results for three possibilities in the table above. Label each column with how you combined the four concentrations in the box provided. Discuss your results below.

8. The phenomenon illustrated in this activity is called *chemical equilibrium*. Equilibrium implies a balance. Explain what is meant by "balance" for this reaction.

9. Write the equilibrium expression, given the following general equation.

$$aA(g) + bB(g) \rightleftharpoons cC(g) + dD(g)$$
CALCULATING THE EQUILIBRIUM CONSTANT FOR A REACTION

Section

- 1. Below are listed three reactions. Associated with each reaction is a 1.0 L container with a particulate level representation of the reaction before the reaction has occurred. To the right is the 1.0 L container with a particulate level representation of the reaction after attaining equilibrium. In each case indicate whether you think the equilibrium constant for the reaction is greater than 1, less than 1 or equal to 1. In each case support your answer with a brief explanation.
 - a. Reaction I : $A_2(g) + B_2(g) \rightleftharpoons 2AB(g)$ (where \bigcirc is A_2 and \bigcirc is B_2)



Is the equilibrium constant for the reaction greater than 1, less than 1 or equal to 1? Explain.

b. Reaction II : $C_2(g) + D_2(g) \rightleftharpoons 2CD(g)$ (where $\bigcirc \bigcirc$ is C_2 and $\bigcirc \bigcirc$ is D_2)



Is the equilibrium constant for the reaction greater than 1, less than 1 or equal to 1? Explain.

c. Reaction III : $X_{2}(g) + Y_{2}(g) \rightleftharpoons 2XY(g)$ (where $\bigcirc \bigcirc$ is X_{2} and \bigcirc is Y_{2})



Is the equilibrium constant for the reaction greater than 1, less than 1 or equal to 1? Explain.

d. If any of the cases (K > 1, K < 1 or K = 1) did not appear in the three examples above, use the space below to draw the before container, and the equilibrium container for the missing case.



Container Before Reaction Started

Container After Reaction Achieves Equilibrium

Explain how your model properly represents the particular case.

2. The following reaction is at equilibrium at a particular temperature

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

and the $[H_2]_{eq} = 0.012$ M, $[I_2]_{eq} = 0.15$ M and $[HI]_{eq} = 0.30$ M. Calculate the magnitude of K_c for the reaction.

- 3. Using the equilibrium constant calculated in 2, calculate the magnitude of the equilibrium constant for the following reactions at the same temperature.
 - a. $2\text{HI}(g) \rightleftharpoons \text{H}_2(g) + \text{I}_2(g)$

b.
$$\frac{1}{2}$$
 H₂(g) + $\frac{1}{2}$ I₂(g) \rightleftharpoons HI(g)

4. The initial concentration of both H_2 and I_2 is 0.250 M. The reaction occurs as shown below,

$$H_{\gamma}(g) + I_{\gamma}(g) \rightleftharpoons 2HI(g)$$

When equilibrium is achieved the concentration of HI is 0.390 M. Calculate the magnitude of $\rm K_c$ for the reaction.

5. A vessel initially has a partial pressure of NO equal to 0.526 atm and a partial pressure of Br_2 equal to 0.329 atm. At equilibrium the partial pressure of Br_2 is 0.203 atm. Calculate K_p for the reaction

 $2NO(g) + Br_2(g) \rightleftharpoons 2NOBr(g)$

CALCULATING THE EQUILIBRIUM CONCENTRATION OF ALL SPECIES

Name

Section

1. Below are 1.0 L containers for the initial and equilibrium condition for the reaction,

 $A_2(g) + D_2(g) \implies 2AD(g)$

Calculate the magnitude of the equilibrium constant for the reaction.



Show work:

2. Set up the ICE table for the following general chemical equation. (Assume the reaction proceeds from left to right to establish equilibrium.)

$$A_2(g) + D_2(g) \rightleftharpoons 2AD(g)$$

3. The equilibrium constant, K_p , for the reaction

$$2 \operatorname{HI}(g) \rightleftharpoons \operatorname{H}_{2}(g) + \operatorname{I}_{2}(g)$$

is 0.0202. If the initial partial pressure of $H_2 = I_2 = 0.350$ atm, calculate the equilibrium partial pressures of all species.

4. The equilibrium constant, K_c , for the reaction

$$PCl_{5}(g) \rightleftharpoons PCl_{3}(g) + Cl_{2}(g)$$

is 33.3 at 760 °C. If 0.400 mol of PCl_5 are placed in a 2.00 liter container, calculate the equilibrium concentrations of all species.

5. The equilibrium constant, K_c , for the reaction

$$PCl_{5}(g) \rightleftharpoons PCl_{3}(g) + Cl_{2}(g)$$

is 33.3 at 760 °C. If 0.400 mol of PCl_5 and 1.0 mol of Cl_2 are placed in a 2.00 liter container, calculate the equilibrium concentrations of all species.

LE CHÂTELIER'S PRINCIPLE

Name

Section

This DCI consists of a series of experiments that involve interaction between you (the student), your instructor and a molecular level simulation.[†] Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ERGBN.htm

1. Open the Graphics Simulation program. Using the data from the Control Bar Region, enter the initial concentration of each substance in the equation below

EXPERIMENT #1:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C		-					
Ending Concentration – E		-					

Click on the Resume and then the Enable Reactions button to begin the reaction. When the reaction appears to be complete, click Pause to stop the action. Record the values of the ending concentrations in the table in Section 1.A. Calculate the change in concentration of each of the substances in the reaction.

Notes, observations, and speculations:

⁺ If you do not have access to this DCI's website link, your instructor will provide you with the data you will need to complete Experiments 1–6.

2. If necessary, click Pause to stop the action. Use the ending concentrations of BG, RG and B from Experiment #1 (Section 1.A.) as the initial concentrations in this experiment. Enter those values in the table below. In the Control Bar Region, add R until its concentration is 2.0 M. Record this initial concentration of R in the table below. Click the Resume button. Use the strip chart to observe how the concentrations of each of the substances change over time. When the reaction appears to be complete, click the Pause button. Record the values of the ending concentrations in this table

EXPERIMENT #2: Increase reactant R to 2.0 M	R	+	BG	\rightleftharpoons	RG	+	В
Initial Concentration – I				_		_	
Concentration Change – C				_		_	
Ending Concentration – E				-		-	

Notes, observations, and speculations:

3. If you moved the strip chart scrollbar in the previous section, shift it back to as far to the right as it will go. Use the ending concentrations of R, RG and B from Experiment #2 as the initial concentrations in this experiment. Enter those values in the table below. In the Control Bar Region, add BG until its concentration is 1.0 M. Record this initial concentration of BG in the table below. Click the Resume button. Use the strip chart to observe how the concentrations of each of the substances change over time. When the reaction appears to be complete, click the Pause button. Record the values of the ending concentrations in this table

EXPERIMENT #3: Increase reactant BG to 1.0 M	R	+	BG	\rightleftharpoons	RG	+	В
Initial Concentration – I						_	
Concentration Change – C							
Ending Concentration – E							

Notes, observations, and speculations:

4. In a manner similar to the previous experiments remove R until its concentration equals 0.75 M. Record the new initial conditions of all substances in the table below. Click the Resume button. Use the strip chart to observe how the concentrations of each of the particles in the sample change over time. When the reaction appears to be complete click the Pause button. Record the values of the ending concentrations in the table and calculate the change in concentration of each of the substances in the reaction.

R	+	BG	\rightleftharpoons	RG	+	В
					_	
					_	
					_	
-	R	R +	R + BG	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

Notes, observations, and speculations:

5. In a manner similar to the previous experiments add RG until its concentration is 2.0 M. Record the new initial conditions of all substances in the table below.

EXPERIMENT #5: Increase product RG to 2.0 M	R	+	BG	\rightleftharpoons	RG	+	В
Initial Concentration – I						_	
Concentration Change – C						_	
Ending Concentration – E							

Notes, observations, and speculations:

6. In a manner similar to the previous experiments remove RG until its concentration is 1.0 M. Record the new initial conditions of all substances in the table below.

EXPERIMENT #6: Decrease product RG to 1.0 M	R	+	BG	\rightleftharpoons	RG	+	В
Initial Concentration – I						_	
Concentration Change – C						_	
Ending Concentration – E						_	

Notes, observations, and speculations:

7. Summarize your observations of Experiments #3 – #6 by completing the table below. As an example, the entries for Experiment #2 have been done for you.

Experiment	Stress	Change in [Reactants]	Change in [Products]	Reaction shift
#2	Add reactant [R]	Concentrations decreased	Concentrations increased	Left to Right
#3				
#4				
#5				
#6				

8. Review the summary of your experimental observations that you prepared in Section IV.A. Write a statement(s) that generalizes how stressing a reaction by adding or removing a reactant or product shifts the chemical reaction.

NON-EQUILIBRIUM REACTION QUOTIENT

Name

Section

1. The reaction

$$H_{2}(g) + I_{2}(g) \rightleftharpoons 2HI(g)$$

occurs in a 1.0 L container at a given temperature. Initially the concentration of $[H_2]$ and $[I_2]$ are both 0.350 M. In the table below are the results of 6 successive measurements where the concentration of each species in the reaction is provided.

Measurement #	[H ₂] (M)	[I ₂] (M)	[HI] (M)	ratio [HI] ² /[H ₂][I ₂]
1	0.350	0.350	0	0
2	0.255	0.255	0.190	
3	0.155	0.155	0.390	
4	0.0900	0.0900	0.520	
5	0.0775	0.0775	0.545	
6	0.0775	0.0775	0.545	

Calculate the magnitude of the reaction quotient, $\frac{\left[\text{HI}\right]^2}{\left[\text{H}_2\right]\left[\text{I}_2\right]}$ for each measurement and enter the value into the appropriate cell in the table above. (Show at least one of the calculations here.)

a. What is happening to the value of the reaction quotient moving from Exp. #1 to Exp. #5?

- b. For Exp. #4 what is the concentration of H_2 and I_2 reacting?
- c. For Exp. #4 what is the concentration of HI formed?
- d. Explain the relationship between the concentration of H_2 and I_2 reacting and the concentration of HI forming.
- e. What is happening in Exp. #5 and #6?

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- f. What is the magnitude of the equilibrium constant for this reaction?
- g. If an Exp. #7 and an Exp. #8 were performed, what would you expect the reaction quotient to be?

2. The reaction

$$NOBr(g) \rightleftharpoons NO(g) + \frac{1}{2}Br_{,(g)}$$

has been carefully studied at 350 °C and the K_c is 0.079. Which direction will the reaction proceed to establish equilibrium under each of the following initial conditions?

a. $[NOBr]_{o} = 0.100 \text{ M} : [NO]_{o} = 0 : [Br_{2}]_{o} = 0$

b.
$$[NOBr]_{o} = 0 : [NO]_{o} = 0.100 \text{ M} : [Br_{2}]_{o} = 0.100 \text{ M}$$

c.
$$[NOBr]_{o} = 0.100 \text{ M} : [NO]_{o} = 0 : [Br_2]_{o} = 0.100 \text{ M}$$

d.
$$[NOBr]_{o} = 0.100 \text{ M} : [NO]_{o} = 0.100 \text{ M} : [Br_{2}]_{o} = 0.100 \text{ M}$$

e. $[NOBr]_{o} = 0.200 \text{ M} : [NO]_{o} = 0.0500 \text{ M} : [Br_{2}]_{o} = 0.100 \text{ M}$

TEMPERATURE DEPENDENCE OF THE EQUILIBRIUM CONSTANT

Name

Section

1. For the reaction

$$2NO_{4}(g) \rightleftharpoons N_{4}(g)$$

the following data was collected for the magnitude of the equilibrium constant at different temperatures. Complete the columns 1/T (K) and ln (K).

Temperature (K)	1/T (K)	К	ln (K)
273.0		72.9	
280.0		38.8	
290.0		16.6	
298.0		8.8	
305.0		5.2	
315.0		2.5	
325.0		1.3	

a. How does the equilibrium constant for this reaction change with temperature?

b. Is the reaction exothermic or endothermic? Explain.

c. What does a plot of ln (K) (y-axis) versus 1/T (x-axis) look like? (Use the graph paper that follows.)

d. If the slope of the line in the plot above is equal to $-\Delta H^{\circ}/R$ (where R is 8.314 J mol⁻¹ K⁻¹.), what is ΔH° for the reaction?

e. Estimate the value of K at 278 K.

f. Estimate the temperature (K) when the equilibrium constant is 100.

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2. In the reaction

$$2NO_2(g) \rightleftharpoons N_2O_4(g)$$

 Δ H = ⁻57.2 kJ mol⁻¹ at 25 °C. The equilibrium constant, K_p, at this temperature is 8.8. Calculate K_p at 0 °C.

3. In the reaction

$$2\mathrm{ICl}(g) \rightleftharpoons \mathrm{I}_2(g) + \mathrm{Cl}_2(g)$$

 Δ H = 26.9 kJ mol⁻¹ at 25 °C. The equilibrium constant, K_c, at this temperature is 4.9 × 10⁻⁶. Calculate K_c at 100 °C.

ARRHENIUS ACIDS [H⁺], [OH⁻], pH AND pOH

Name

Section

- 1. a. Hydrochloric acid, HCl(*aq*), breaks up into ions (a cation and an anion) in a water solution. Write a chemical equation that represents this process.
 - b. Nitric acid, HNO₃(*aq*), also breaks up into ions (a cation and an anion) in a water solution. Write a chemical equation that represents this process.
 - c. Write a definition describing what happens to acids when they interact with water.
- 2. a. Sodium hydroxide, NaOH, breaks up into ions (a cation and an anion) in water solution. Write a chemical equation that represents this process.
 - b. Potassium hydroxide, KOH, also breaks up into ions (a cation and an anion) in water solution. Write a chemical equation that represents this process.
 - c. NaOH and KOH are classified as bases. Write a definition describing what happens to bases when they interact with water.

3. Defining acids and bases in terms of the characteristic ions that are released in water solution is the Arrhenius Theory of acids and bases. In the space below, list some examples of Arrhenius acids and Arrhenius bases.

Arrhenius Acids	Arrhenius Bases

4. a. Draw the Lewis structure for water, H₂O.

b. Describe how water might break up into ions. Write a chemical equation for this process. How is water related to Arrhenius acids and bases?

c. Unlike HCl, only a small fraction of water molecules break up into ions. The equilibrium constant for water dissociating into ions is 1.0×10^{-14} . Write an equilibrium expression for the dissociation of water. What would be the concentration of each of the ions in a pure sample of water?

- 5. a. pH is a measure of the [H⁺]. The pH of pure water = 7. Write an equation that relates pH to [H⁺] by comparing 7 with the [H⁺] of pure water.
 - b. Use Le Châtelier's Principle to predict what would happen to the [H⁺] and [OH⁻] of a water sample if you added HCl to it. What would happen to the value of the pH?
 - c. Use Le Châtelier's Principle to predict what would happen to the [H⁺] and [OH⁻] of a water sample if you added NaOH to it. What would happen to the value of the pH?
 - d. pOH is a measure of the [OH⁻]. The pOH of pure water = 7. Write an equation that relates pOH to [OH⁻] by comparing 7 with the [OH⁻] of pure water.
- 6. a. The [H⁺] in a particular aqueous solution is 1.0×10^{-4} M. Calculate the [OH⁻] for this solution.
 - b. The $[OH^-]$ in a particular aqueous solution is 1.0×10^{-5} M. Calculate the $[H^+]$ of this solution.
 - c. The [H⁺] in a particular aqueous solution is 6.0 M. Calculate the [OH⁻] of this solution.

- 7. a. Calculate the pH and pOH of a solution with a $[H^+] = 3.68 \times 10^{-8} M$.
 - b. Calculate the $[H^+]$ and $[OH^-]$ of a solution with a pH = 4.22.

BRØNSTED-LOWRY ACID/BASE THEORY

Name

Section

1. NH₃(*aq*) solutions have pH>7. How would you characterize such a solution? What ion would you expect to be present? Where might that ion come from?

2. Knowing that $NH_3(aq)$ solutions have pH>7, complete the following chemical equation.

$$\rm NH_3(aq) + H_2O \rightarrow$$

Describe the role that water plays in this reaction. How does the water interact with NH₃?

3. Describe what happens to the NH₃ in this reaction and what substance is produced.

The relationship between NH₃ and its product is said to be a conjugual one. The substances are said to be conjugates of each other. What is the conjugate acid for water? What is its conjugate base?

4. The transfer of a proton (H⁺) from acid to conjugate base characterizes the Brønsted-Lowry Theory of acids and bases. Identify differences between the Brønsted-Lowry Theory and the Arrhenius Theory. Identify examples of Brønsted-Lowry bases that are not also Arrhenius bases. Identify examples of Brønsted-Lowry bases that are not also Arrhenius bases. Identify examples of Brønsted-Lowry acids that are not also Arrhenius acids.

- 5. Identify the conjugate bases for each of the following acids.
 - a. NH_4^+
 - b. H₃PO₄
 - c. H₂O
- 6. Identify the conjugate acid for each of the following bases.
 - a. Br-
 - b. HSO₄-
 - c. H₂O

ACIDS, BASES AND pH

Name

Section

1. a. Go to http://introchem.chem.okstate.edu/DCICLA/ph_meter.html.[†] Adjust the "solutions" settings to "acid" (or "base") and the concentration to 10 x 10⁻² M, choose the acid (or base) and complete the following table.

Solution	рН	Equilibrium [H ⁺] or [OH ⁻]
0.100 M HCI		
0.100 M HNO ₃		
0.100 M H ₂ SO ₄		
0.100 M HC ₂ H ₃ O ₂		
0.100 M NaOH		
0.100 M NH ₃		

- b. How does the measured concentration of the H⁺ compare to the concentration of HCl?
- c. This relationship is characteristic of a strong acid. Briefly describe the qualitative relationship between the concentration of a strong acid and the extent of the dissociation of the acid into its ions.
- d. How does the measured concentration of the OH- compare to the concentration of NaOH?

[†] If you do not have access to this DCI's website link, your instructor will provide you with the data you will need.

e. This relationship is characteristic of a strong base. Briefly describe the qualitative relationship between the concentration of a strong base and the extent of the dissociation of the base into its ions.

f. Calculate the pH of a 0.450 M HCl solution.

g. Calculate the pH of a 0.710 M KOH solution.

STRONG ACIDS AND THE EQUILIBRIUM CONSTANT

Name

Section

1. The chemical equation which describes how the strong acid HCl dissociates in aqueous solution is,

 $HCl(aq) \rightleftharpoons H^{+}(aq) + Cl^{-}(aq)$

a. In the data you obtained earlier (Acids, Bases and pH, pg. 55), the initial concentration of HCl is 0.100 M. In the space provided below (ICE Table), enter the initial concentration of HCl, H⁺ and Cl⁻. Based on the measured pH of this solution, calculate and enter the equilibrium concentration of H⁺.

- b. Calculate the change in $[H^+]$.
- c. Using the balanced chemical equation and the calculated change in [H⁺], calculate the change in [HCl] and [Cl⁻].
- d. Calculate the equilibrium concentration of HCl(aq) and $Cl^{-}(aq)$.
- e. Estimate the equilibrium constant for the dissociation of HCl(*aq*).

WEAK ACIDS AND THE EQUILIBRIUM CONSTANT

Name

Section

59

1. The chemical equation which describes how the weak acid HC₂H₃O₂ dissociates in aqueous solution is,

$$\mathrm{HC}_{2}\mathrm{H}_{3}\mathrm{O}_{2}(aq) \rightleftharpoons \mathrm{H}^{+}(aq) + \mathrm{C}_{2}\mathrm{H}_{3}\mathrm{O}_{2}^{-}(aq)$$

a. In the data you obtained earlier (Acids, Bases and pH, pg. 55), the initial concentration of HC₂H₃O₂ is 0.100 M. In the space provided below (ICE Table), enter the initial concentration of HC₂H₃O₂, H⁺ and C₂H₃O₂⁻. Based on the measured pH of this solution, calculate and enter the equilibrium concentration of H⁺.

$$HC_2H_3O_2(aq) \rightleftharpoons H^+(aq) + C_2H_3O_2^-(aq)$$



- b. Calculate the change in $[H^+]$.
- c. Using the balanced chemical equation and the calculated change in [H⁺], calculate the change in [HC₂H₃O₂] and [C₂H₃O₂⁻].
- d. Calculate the equilibrium concentration of $HC_2H_3O_2(aq)$ and $C_2H_3O_2^-(aq)$.

- e. Estimate the equilibrium constant for the dissociation of $HC_2H_3O_2(aq)$.
- f. Calculate the magnitude of the equilibrium constant for benzoic acid, $HC_7H_5O_2$, if a 0.100 M solution has a pH = 2.59.

g. Calculate the magnitude of the equilibrium constant for an aqueous solution of ammonia, if a 0.100 M solution has a pH = 11.13.

h. Calculate the pH of a solution which is 0.53 M $HC_6H_4NO_2$ (nicotinic acid). (K_a = 1.4 × 10⁻⁵)

i. Calculate the pH of a solution which is 0.712 M CH₃NH₂ (methylamine). ($K_b = 4.4 \times 10^{-4}$)

POLYPROTIC ACIDS

Name

Section

- 1. Refer to the data you obtained earlier (Acids, Bases and pH, pg. 55). Compare the pH and [H⁺] of H₂SO₄ with that of HCl and HNO₃. How do you account for any differences?
- 2. H_2SO_4 is a polyprotic acid. What does this term mean? Write the equations which describe the stepwise dissociation of H_2SO_4 .
- 3. Carbonic acid, H_2CO_3 , is a diprotic acid.
 - a. Write the two dissociation reactions showing its diprotic behavior.
 - b. If the initial concentration of H_2CO_3 is 0.100 M, calculate [H⁺]. In your calculation, assume only the first dissociation occurs. (Note: The equilibrium constant for the first dissociation, K_{a1} , is 4.3×10^{-7} .)

c. Now consider the second dissociation equation for which $K_{a2} = 5.6 \times 10^{-11}$. What is the initial concentration of $[HCO_3^-]$? What is the initial concentration of $[H^+]$? Calculate the final $[H^+]$ assuming the second dissociation occurs.

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SALTS I

Name	Section

- 1. Define the term *salt*.
- 2. Go to http://introchem.chem.okstate.edu/DCICLA/ph_meter.html.[†] Adjust the "solutions" settings to "salts 1" and the concentration to 10×10^{-2} M, choose the salt and complete the following table.

Solution	рН	Equilibrium [H⁺] or [OH⁻]	Acidic, basic or neutral
0.100 M NaCl			
0.100 M NaC ₂ H ₃ O ₂			
0.100 M NH ₄ Cl			

3. Predict the product of the neutralization reactions,

$$\begin{split} &\mathrm{HCl}(aq) + \mathrm{NaOH}(aq) \rightarrow \\ &\mathrm{HC}_{2}\mathrm{H}_{3}\mathrm{O}_{2}(aq) + \mathrm{NaOH}(aq) \rightarrow \\ &\mathrm{HCl}(aq) + \mathrm{NH}_{3}(aq) \rightarrow \end{split}$$

4. In general, what is the acid–base property of any salt formed in the reaction between a strong acid and a strong base?

[†] If you do not have access to this DCI's website link, your instructor will provide you with the data you will need.

- 5. In general, what is the acid–base property of any salt formed in the reaction between a strong acid and a weak base?
- 6. In general, what is the acid-base property of any salt formed in the reaction between a weak acid and a strong base?
- 7. a. Write the dissociation equation which describes what happens when $NaC_{2}H_{3}O_{2}(s)$ is added to water.
 - b. Write the equation that describes the acidic character of $Na^+(aq)$. Write the equilibrium expression and estimate K_a for $Na^+(aq)$.
 - c. Write the equation which describes the basic character of $C_2H_3O_2^-(aq)$. Write the equilibrium expression and calculate the K_b for $C_2H_3O_2^-(aq)$.
 - d. Which of the two ions, $Na^+(aq)$ or $C_2H_3O_2^-(aq)$, affects the pH of the solution? Explain why.
 - e. Predict the products when KCN(*s*) is added to water. Will the pH of the solution formed when the salt is added to water be greater or less than 7?

- 8. a. Write the dissociation equation which describes what happens when $NH_4Cl(s)$ is added to water.
 - b. Write the equation which describes the acidic character of $NH_4^+(aq)$. Write the equilibrium expression and calculate K_a for $NH_4^+(aq)$.
 - c. Write the equation which describes the basic character of $Cl^{-}(aq)$. Write the equilibrium expression and estimate K_b for $Cl^{-}(aq)$.
 - d. Which of the two ions, $NH_4^+(aq)$ or $Cl^-(aq)$, affects the pH of the solution? Explain why.
 - e. Predict the products when $CH_3NH_3NO_3(s)$ is added to water. Will the pH of the solution formed when the salt is added to water be greater or less than 7?
SALTS II

Name

Section

1. Calculate the pH of a 0.700 M NaC₂H₃O₂. K_a(HC₂H₃O₂) = 1.8×10^{-5} .

2. Calculate the pH of a 0.392 M CH₃NH₃NO₃. K_b (CH₃NH₂) = 4.4 × 10⁻⁴.

THE COMMON ION EFFECT

Name

Section

1. a. Transfer the pH data you obtained earlier (Acids, Bases and pH, pg. 55 and Salts I, pg. 63) for 0.100 M HC₂H₃O₂ and for 0.100 M NaC₂H₃O₂ and add this data to the following table.

Solution	рН
0.100 M HC ₂ H ₃ O ₂	
0.100 M NaC ₂ H ₃ O ₂	
0.100 M HC ₂ H ₃ O ₂ /	
0.100 M NaC ₂ H ₃ O ₂	

- b. Write the equilibrium expression for the hydrolysis (reaction with water) of the weak acid $HC_2H_3O_2$. What is the K_a for this reaction? Use Le Châtelier's Principle to predict what would happen if you added $NaC_2H_3O_2$ to this solution.
- c. Go to http://introchem.chem.okstate.edu/DCICLA/pHbuffer20.html⁺and complete the previous table for 0.100 M HC₂H₃O₂ / 0.100 M NaC₂H₃O₂. Compare the pH of this solution with your prediction in the previous question.

⁺ If you do not have access to this DCI's website link, your instructor will provide you with the data you will need.

- d. Provide an example of an aqueous solution containing a weak base and the soluble salt of the base.
- e. How is the extent of dissociation of a weak acid or weak base affected by the presence of its soluble salt?

2. Calculate the pH of a solution which is 0.53 M HC₆H₄NO, and 0.50 M NaC₆H₄NO,

3. Calculate the pH of a solution which is 0.245 M NH₃ and 0.245 M NH₄NO₃.

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NEUTRALIZATION REACTIONS

Name

Section

- 1. Write the ionic and net ionic equations for the following reactions, the equilibrium expression for the net ionic equation, and determine the magnitude of the equilibrium constant.
 - a. $HCl(aq) + NaOH(aq) \rightarrow H_2O(l) + NaCl(aq)$

b. $HC_2H_3O_2(aq) + KOH(aq) \rightarrow H_2O(l) + KC_2H_3O_2(aq)$

c. $HNO_3(aq) + NH_3(aq) \rightarrow NH_4NO_3(aq)$

What is the general conclusion which can be made from the magnitude of the equilibrium constant in all three examples above?

TITRATION BETWEEN A STRONG ACID AND A STRONG BASE

Name

Section

1. Qualitatively, describe how the pH of a solution of a strong acid changes when a solution of strong base is added to it.

- a. A titration is performed by adding 0.600 M KOH to 40.0 mL of 0.800 M HCl.
 - i. Calculate the pH before addition of any KOH.

ii. Calculate the pH after the addition of 5.0 mL of the base.

ii. (Continued)

Calculate the pH after the addition of 20.0 mL of the base.

Calculate the pH after the addition of 40.0 mL of the base.

Calculate the pH after the addition of 52.0 mL of the base.

Calculate the pH after the addition of 53.0 mL of the base.

iii. Calculate the volume of base needed to reach the equivalence point.

iv. What is the pH at the equivalence point?

v. Calculate the pH after adding 5.00 mL of KOH past the equivalence point.

- 2. Using the designated space below sketch the titration curve for each of the following cases.
 - a. 50.0 mL of 0.100 M KOH is added to 50.0 mL of 0.100 M HCl
 - b. 50.0 mL of 0.00100 M NaOH is added to 50.0 mL of 0.00100 M HCl

Plot both curves on the graph below.



c. Describe similarities and differences of the two curves.

TITRATION BETWEEN A WEAK ACID AND A STRONG BASE

Name

Section

1. a. Qualitatively, describe how the pH of a solution of a weak acid changes when a solution of strong base is added to it.

- b. A titration is performed by adding 0.200 M NaOH to 24 mL of 0.350 M HOCl.
 - i. Calculate the pH before addition of any NaOH.

ii. Calculate the pH after the addition of 5.0 mL of the base.

Calculate the pH after the addition of 15.0 mL of the base.

Calculate the pH after the addition of 25.0 mL of the base.

Calculate the pH after the addition of 35.0 mL of the base.

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Calculate the pH after the addition of 40.0 mL of the base.

iii. Calculate the volume of base needed to reach the equivalence point.

iv. What is the pH at the equivalence point?

v. Calculate the pH after adding 5.00 mL of NaOH past the equivalence point.

- 2. Using the designated space below, draw the titration curve for each of the following cases.
 - a. 50.0 mL of 1.00 M NaOH is added to 50.0 mL of 1.00 M $HC_2H_3O_2$
 - b. 50.0 mL of 0.0100 M NaOH is added to 50.0 mL of 0.0100 M $HC_2H_3O_2$



c. Describe similarities and differences of the two curves.

INTRODUCTION TO BUFFERS

Name

Section

1. a. A buffer solution is constructed from a weak acid and its conjugate weak base such that both are present in substantial concentrations. List two example buffer solutions. Write a chemical equation that represents the equilibrium on which the buffer is based.

b. Use one of your examples from the previous question to describe how the pH of the solution would be affected by the addition of a small amount of acid. (Hint: use Le Châtelier's Principle in your explanation.)

c. Use one of your examples from the previous question to describe how the pH of the solution would be affected by the addition of a small amount of base. (Hint: use Le Châtelier's Principle in your explanation.)

d. Explain how the behavior you described in the previous questions would have been different with an unbuffered solution.

e. Explain how a buffered solution consisting of a weak acid and a weak base could be constructed from a weak acid and a strong base or a weak base and a strong acid. Write a chemical equation representing how this can be done.

- 2. Complete the following problems:
 - a. Calculate the pH of a solution prepared by mixing 20.0 mL of 0.300 M $HC_2H_3O_2$ with 20.0 mL of 0.350 M $NaC_2H_3O_2$.

b. Specify the reagents and the specific concentrations of each reagent needed to prepare a buffer solution which would have a pH of 4.19.

BUFFERS

Name	Section

1. a. Calculate the pH of a solution prepared by mixing 20.0 mL of 0.300 M HC₂H₃O₂ with 20.0 mL of 0.350 M NaC₂H₃O₂.

b. Calculate the pH after adding 0.0000200 moles of NaOH to this buffer.

c. Calculate the pH after adding 0.0000200 moles of HCl to a new sample of this buffer.

d. Calculate the pH before and after adding 0.0000200 moles of HCl to 20 mL of water.

e. Compare the original pH of the buffers with the pH after the acid and base have been added. What is a characteristic of buffer solutions when compared to unbuffered solutions? How might these kinds of solutions be useful?

PRECIPITATION AND SOLUBILITY

Name

Section

1. Using the solubility table below predict whether the following compounds are soluble or insoluble in water.

lon Solubility Exceptions				
1011	Solubility	Exceptions		
NO ₃ -	soluble	none		
ClO ₄ -	soluble	none		
Cl-	soluble	except Ag ⁺ , Hg ₂ ²⁺ , *Pb ²⁺		
I-	soluble	except Ag ⁺ , Hg ₂ ²⁺ , Pb ²⁺		
SO ₄ ²⁻	soluble	except Ca ²⁺ , Ba ²⁺ , Sr ²⁺ , Hg ²⁺ , Pb ²⁺ , Ag ⁺		
CO ₃ ²⁻	insoluble	except Group IA and NH ₄ ⁺		
PO ₄ ³⁻	insoluble	except Group IA and NH ₄ ⁺		
-OH	insoluble	except Group IA, *Ca ²⁺ , Ba ²⁺ , Sr ²⁺		
S ²⁻	insoluble	except Group IA, IIA and NH ₄ ⁺		
Na ⁺	soluble	none		
NH_{4}^{+}	soluble	none		
K ⁺	soluble	none		
		*slightly soluble		

Solubility Table

a. AgI

b. $(NH_4)_2SO_4$

c. Cu(OH)₂

- 2. Complete and balance the following reactions. Identify all products, phases as either (g)as, (l)iquid, (s)olid or (aq)ueous. If no reaction occurs, write NR.
 - a. Na₂SO₄(*aq*) + Ba(NO₃)₂(*aq*) \rightarrow
 - b. $\operatorname{AgNO}_{3}(aq) + \operatorname{KCl}(aq) \rightarrow$
 - c. $Fe(NO_3)_3(aq) + HCl(aq) \rightarrow$
 - d. $2NH_4I(aq) + Pb(NO_3)_2(aq) \rightarrow$
- 3. Write the equilibrium expression for the reaction described by the general solubility equation below,

 $M_n X_m(s) \rightleftharpoons n M^{m_+}(aq) + m X^{n_-}(aq)$

4. Define the term *solubility product constant*.

If the value of the equilibrium constant (K_{sp} —also called the solubility product) for the above equation is of the order of 10⁻⁸, what does this tell you about the solubility of $M_{p}X_{m}$?

5. Complete the following problem:

Calculate the K_{sp} for Bi(OH), if 1.1×10^{-8} moles of Bi(OH), dissolve in 1.0 liter of water to form a saturated solution.

SOLUBILITY EQUILIBRIA PROBLEMS

Name

Section

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1. Calculate the solubility of $BaSO_4$ in H_2O . $K_{sp} = 1.1 \times 10^{-10}$.

2. Calculate the solubility of $BaSO_4$ in 0.100 M Na_2SO_4 .

- 3. A 50.0 mL sample of 0.0152 M Na_2SO_4 is added to 50.0 mL of 0.0125 M $Ca(NO_3)_2$.
 - a. Should the precipitation of CaSO₄ occur?
 - b. What % of the Ca^{2+} will precipitate?

4. a. Under what circumstances will the solubility of an ionic compound be dependent on the pH of the solution?

b. Give two examples of ionic compounds that are more soluble in acidic solutions than basic solutions.

c. Give two examples of ionic compounds that are more soluble in basic solutions than acidic solutions.

ENTHALPY AND THE FIRST LAW

Name

Section

- 1. Energy in the form of heat can be either released (exothermic) or absorbed (endothermic) in a chemical reaction. This heat, called the enthalpy, is a driving force for chemical reactions. Predict which of the following spontaneous reactions are exothermic and which are endothermic.
 - a. $H_2O(l) \rightarrow H_2O(g)$ @25 °C
 - b. $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$
 - c. $Ba(OH)_{2} \bullet 8H_{2}O(s) + 2NH_{4}Cl(s) \rightarrow BaCl_{2}(aq) + 10H_{2}O(l) + 2NH_{3}(aq)$

d.
$$H_2(g) + \frac{1}{2}O_2(g) \to H_2O(l)$$
 or (g)

- e. $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$
- f. $\operatorname{Al}(s) + \frac{3}{2}\operatorname{Br}_2(l) \to \operatorname{AlBr}_3(s)$
- 2. A formation reaction is a chemical reaction depicting the formation of one mole of a substance from its naturally occurring elemental sources. Which of the reactions in question 1 are formation reactions?

3. A table of heats (enthalpies) of formation (ΔH°_{f}) for selected substances is at the end of this DCI. Write the mathematical equation that relates the standard heat of reaction to the heats of formation of the reactants and products of the chemical reaction.

4. Calculate the heats of reaction for the chemical reactions in question 1.

5. The natural tendency for spontaneous chemical reactions is to release heat. Is the enthalpy an absolute predictor of spontaneity? Defend your answer.

Thermodynamic Values (25°C)

Substance and	$\Delta H^0_{\ f}$	$\Delta G^0_{\ f}$	S^0	Substance and	$\Delta H^0_{~f}$	$\Delta G^0_{\ f}$	S^0
State	$\begin{pmatrix} kJ \end{pmatrix}$	$\begin{pmatrix} kJ \end{pmatrix}$	$\left(J \right)$	State	$\begin{pmatrix} kJ \end{pmatrix}$	$\begin{pmatrix} kJ \end{pmatrix}$	$\left(J \right)$
	$\left(\frac{1}{\text{mol}}\right)$	$\left(\frac{1}{\text{mol}}\right)$	$\left(\overline{\mathrm{K}\cdot\mathrm{mol}}\right)$		$\left(\frac{1}{\text{mol}}\right)$	$\left(\frac{1}{\text{mol}}\right)$	$\left(\overline{\mathbf{K}\cdot\mathrm{mol}}\right)$
Aluminum				Iodine			
AlBr ₂ (s)	-526.3	-505	184	I,(s)	0	0	116.7
Al(s)	0	0	28.32	I,(g)	62.25	19.37	260.57
				HI(g)	25.94	1.30	206.3
Barium							
BaCl,(aq)	-872	-823	123	Magnesium			
Ba(OH), ·8H, O(s)	-3342	-2793	427	Mg(s)	0	0	33
				$Mg^{2+}(aq)$	-492	-456	-118
Bromine				MgO(s)	-601	-569	26.9
Br ₂ (l)	0	0	152.231				
BrCl(g)	14.64	-0.96	239.99	Oxygen			
				O ₂ (g)	0	0	205
Carbon				O(g)	249	232	161
C(s) (graphite)	0	0	6	$O_3(g)$	143	163	239
C(s) (diamond)	2	3	2				
CO(g)	-110.5	-137	198	Nitrogen			
CO,(g)	-393.5	-394	214	N,(g)	0	0	192
$CH_4(g)$	-75	-51	186	$NCl_{2}(g)$	230	271	-137
CH ₃ OH(g)	-201	-163	240	$NF_3(g)$	-125	-83.6	-139
CH ₃ OH(l)	-239	-166	127	NH ₃ (g)	-46	-17	193
H,CO(g)	-116	-110	219	$NH_3(aq)$	-80	-27	111
HCOOH(g)	-363	-351	249	NH,CONH,(aq)	?	?	174
HCN(g)	135.1	125	202	NO(g)	90	87	211
C,H,(g)	227	209	201	NO,(g)	34	52	240
$C_{2}H_{4}(g)$	52	68	219	$N_{2}O(g)$	82	104	220
CH ₃ CHO(g)	-166	-129	250	$N_2O_4(g)$	10	98	304
C,H,OH(l)	-278	-175	161	$N_2O_5(g)$	-42	134	178
$C_2H_6(g)$	-84.7	-32.9	229.5	N,H,CH,(l)	54	180	166
$C_3H_6(g)$	20.9	62.7	266.9	$HNO_3(aq)$	-207	-111	146
$C_{3}H_{q}(g)$	-104	-24	270	$HNO_{3}(l)$	-174	-81	156
				NH ₄ Cl(s)	-314	-201	95
Chlorine				$NH_4ClO_4(s)$	-295	-89	186
$\operatorname{Cl}_{2}(g)$	0	0	222.957				
$Cl_2(aq)$	-23	7	121	Silver			
$Cl^{-}(aq)$	-167	-131	57	Ag(s)	0	0	42.6
HCl(g)	-92	-95	187	$Ag^{+}(aq)$	105.6	77.1	72.7
				AgBr(s)	-100.4	-96.9	107.1
Fluorine				AgCl(s)	-127.1	-109.8	96.2
$F_2(g)$	0	0	203				
$F^{-}(aq)$	-333	-279	-14	Sulfur			
HF(g)	-271	-273	174	S(rhombic)	0	0	31.8
				S(monocl)	0.3	0.1	32.6
Hydrogen				SO,(g)	-296.8	-300.2	248.8
H,(g)	0	0	131	$SO_3(g)$	-395.7	-371.1	256.3
H(g)	217	203	115	H,S(g)	-20.17	-33.0	205.6
$H^+(aq)$	0	0	0				
OH ⁻ (aq)	-230	-157	-11	Titanium		I	
H,O(<i>l</i>)	-286	-237	70	TiCl ₄ (g)	-763	-727	355
H,O(g)	-242	-229	189	$TiO_{2}(s)$	-945	-890	50
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SPONTANEITY AND ENTROPY

Name

Section

- 1. Entropy (S) is a second driving force for chemical reactions. Define the term *entropy*. How is the sign of Δ S for a chemical reaction interpreted?
- 2. Predict which of the following spontaneous reactions increase the entropy.
 - a. $H,O(l) \rightarrow H,O(g)$ @25 °C
 - b. $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$
 - c. $Ba(OH)_2 \bullet 8H_2O(s) + 2NH_4Cl(s) \rightarrow BaCl_2(aq) + 10H_2O(l) + 2NH_3(aq)$
 - d. $H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$ or (g)
 - e. $\operatorname{CH}_4(g) + 2\operatorname{O}_2(g) \rightarrow \operatorname{CO}_2(g) + 2\operatorname{H}_2\operatorname{O}(g)$
 - f. $\operatorname{Al}(s) + \frac{3}{2}\operatorname{Br}_2(l) \to \operatorname{AlBr}_3(s)$
- 3. A table of absolute entropies (S°) for selected substances is at the end of this DCI. Identify differences between S° and ΔH°_{f} as thermodynamic values.

- 4. Write the mathematical equation that relates the standard entropy change in a chemical reaction to the absolute entropy of the reactants and products.
- 5. Calculate the change in entropy (ΔS°_{rxn}) for the chemical reactions in question 2.
- 6. The natural tendency for spontaneous chemical reactions is to increase entropy. Is the entropy an absolute predictor of spontaneity? Defend your answer.
- 7. Predict whether the entropy of the system increases, remains constant or decreases when the following processes occur. Explain your reasoning.
 - a. Ice melts at 0 °C.
 - b. A precipitate forms in aqueous solution.
 - c. A solid dissolves in water.
 - d. A gas condenses to a liquid.

Thermodynamic Values (25°C)

State kJ (kJ) (kJ) <th< th=""><th>Substance and</th><th>ΔH^0_{f}</th><th>ΔG^0_{f}</th><th>S^0</th><th>Substance and</th><th>ΔH^0_{f}</th><th>ΔG^0_{f}</th><th>S^{0}</th></th<>	Substance and	ΔH^0_{f}	ΔG^0_{f}	S^0	Substance and	ΔH^0_{f}	ΔG^0_{f}	S^{0}
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	State	(kJ)	(kJ)	(J)	State	(kJ)	(kJ)	(\mathbf{I})
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	State	$\left(\frac{1}{\text{mol}}\right)$	$\left(\frac{1}{\text{mol}}\right)$	$\left \frac{1}{K \cdot mol} \right $	State	$\left(\frac{1}{\text{mol}}\right)$	$\left(\frac{1}{\text{mol}}\right)$	$\left \frac{1}{K \cdot mol} \right $
Autminum Malling (b) (b) (b) (c) (c) (c) (c) (c) (c) (c) (c) (c) (c	A 1	(1101)	(1101)		To d'une	(1101)	(1101)	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Aluminum AlDr. (.)	5262	505	104		0	0	1167
Al(f) 0 0 2.8.2 I,Q 0.2.3 19.37 200.3 Barium HI(g) 25.94 1.30 206.3 BaCl _{(iag}) -872 -823 123 Magnesium BaCl _{(iag}) -3342 -2793 427 Mg(\circ) 0 0 33 BaCl _{(iag}) -492 -456 -118 Mg(\circ) -601 -569 26.9 Br,(i) 0 0 152.231 Mg(\circ) 0 0 205 Carbon O.g(φ 0 0 0 205 23.9 C 143 163 239 Co(g) -110.5 -137 198 Nitrogen -125 83.6 -139 CO(g) -110.5 -394 214 N.(φ 20 0 0 192 CH,OH(g) -201 -166 127 NH(φ -46 -17 193 I,CO(g) -116 110 219 NG(φ	$\frac{\text{Aldr}_{3}(s)}{\text{Al}(s)}$	-520.5	-505	184	$\mathbf{I}_{2}(s)$	0	10.27	2(0.57
Barium 10(g) 23.94 1.50 2005 Barlum BaCl_(aq) -872 -823 123 Magnesium 3 Ba(DI), 8H, O(g) -3342 -2793 427 Mg(g) 0 0 33 Bar(mine Mg(g) -400 -569 26.9 118 Br(d) 0 0 152.231 -601 -569 26.9 Br(d) 14.64 -0.96 239.90 Oxgern - 0(g) 249 232 161 C(g) (graphite) 0 0 6 Oxgern - - CO(g) 143 133 239 CO(g) -110.5 -137 198 Nitrogen - <t< td=""><td>AI(s)</td><td>0</td><td>0</td><td>28.32</td><td>$I_2(g)$</td><td>02.25</td><td>19.37</td><td>200.57</td></t<>	AI(s)	0	0	28.32	$I_2(g)$	02.25	19.37	200.57
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Darium					23.94	1.50	200.5
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	BaCl (aa)	872	873	123	Magnacium			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\frac{\text{DaCl}_2(uq)}{\text{R}_2(\Omega \Pi) \text{ end} \Omega(q)}$	-0/2	-623	123	Magnesium	0	0	2.2
Bromine Img (q_2) -192 -103 -116 Br, (l) 0 0 152.231 -601 -569 26.9 Br,(l) 14.64 -0.96 239.99 Oxygen - - Br(l) 0 0 6 O,(g) 0 0 205 Carbon 0 0 6 O,(g) 143 163 239 C(g) (graphite) 0 0 6 O,(g) 143 163 239 C(g) -110.5 -137 198 Nitrogen -	$\frac{\text{Da}(\text{O}\Pi)_2 \cdot \text{o}\Pi_2 \text{O}(s)}{1}$	-3342	-2/93	427	Mg(s)	402	156	110
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Promino				Mg(uq)	-+92	-+30	26.0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Br (1)	0	0	152 221	NigO(3)	-001	-309	20.9
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\frac{\mathrm{Dr}_2(l)}{\mathrm{Br}\mathrm{Cl}(\alpha)}$	14.64	0.06	230.00	Owigen			
Carbon $O_{(g)}$ 249 232 161 C(g) (graphite) 0 0 6 $O_1(g)$ 143 163 239 C(g) (diamond) 2 3 2	bi Ci(g)	14.04	-0.90	239.99	O_{xygen}	0	0	205
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Carbon				$O_2(g)$	240	232	161
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C(s) (graphite)	0	0	6	O(g)	143	163	230
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C(s) (graphic)	2	3	2	0,0	175	105	237
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C(s) (diamond)		_137	108	Nitrogen			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	CO(g)	303 5	304	214	N (c)	0	0	102
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$CU_2(g)$	-373.3	-377	186	$N_2(g)$	230	271	137
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$CH_4(g)$ CH OH(g)	-75	-163	240	NE (g)	_125	-83.6	_130
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	CH OH()	230	166	127	NH (c)	46	-05.0	103
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	H CO(q)	-239	-110	210	NH (aa)		-17	175
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$H_2CO(g)$	-363	_351	217	NH CONH (ag)	-00 c	-27 C	174
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	HCN(g)	135.1	125	247	$N\Omega(a)$	90		211
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C H (g)	227	209	202	NO(g)	34	52	240
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_2\Pi_2(g)$	52	68	201	$NO_2(g)$ NO(g)	82	104	270
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_2 \Pi_4(g)$ CH CHO(g)	-166	_129	217	$N_{2}O(g)$	10	08	304
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		_278	_175	161	$N_2O_4(g)$	-42	134	178
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C H (a)	_84 7	_32.9	229.5	N H CH (l)	54	180	166
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$C_2 \Pi_6(g)$	20.9	62.7	227.5	HNO(aa)	_207	_111	146
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C_{3}\Pi_{6}(g)$	_104	_24	270	$\frac{11100_3(uq)}{1100_3(uq)}$	_174		156
Chlorine $HI4_4A(g)$ JAT LSA JS $Cl_1(g)$ 0 0 222.957 -295 -89 186 $Cl_1(aq)$ -23 7 121 Silver - - $Cl^-(aq)$ -167 -131 57 Ag(s) 0 0 42.6 HCl(g) -92 -95 187 Ag*(aq) 105.6 77.1 72.7 Image: Close -100.4 -96.9 107.1 - - AgBr(s) -100.4 -96.9 107.1 Fluorine AgCl(s) -127.1 -109.8 96.2 -		101	21	270	NH Cl(s)	_314	-201	95
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Chlorine				NH ClO (s)	_295	_89	186
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Cl(a)	0	0	222 957		275	07	100
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$Cl_2(g)$	-23	7	121	Silver			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$C^{1}(aq)$	-167	-131	57	Ag(s)	0	0	42.6
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	HCl(a)	_92	_95	187	$A\sigma^+(aa)$	105.6	77.1	72.7
Fluorine AgCl(s) -10011 7000 10011 $F_2(g)$ 0 0 203 -127.1 -109.8 96.2 $F_2(g)$ 0 0 203 -		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	75	107	$\operatorname{AgBr}(s)$	-100.4	-96.9	107.1
Figs (g) 0 0 203 12/12 10/13 701 F_j(g) 0 0 203 Sulfur 10/13 701 F(aq) -333 -279 -14 Sulfur HF(g) -271 -273 174 S(rhombic) 0 0 31.8 HYdrogen S(monocl) 0.3 0.1 32.6 Hydrogen SO ₂ (g) -296.8 -300.2 248.8 H ₂ (g) 0 0 131 SO ₃ (g) -395.7 -371.1 256.3 H(g) 217 203 115 H ₂ S(g) -20.17 -33.0 205.6 H*(aq) 0 0 0 0 0 0 0 0 OH ⁺ (aq) -230 -157 -11 Titanium -20.17 -33.0 205.6 H_2O(l) -286 -237 70 TiCl ₄ (g) -763 -727 355 H_O(g) -242 -229 189 TiO ₂ (s) -945 -890 50	Fluorine				AgCl(s)	-127.1	-109.8	96.2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$F(\sigma)$	0	0	203		12/11	107.0	/0.2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$F^{-}(aa)$	-333	-279	_14	Sulfur			
Hydrogen SO,(g) -296.8 -300.2 248.8 H_2(g) 0 0 131 SO_3(g) -296.8 -300.2 248.8 H_2(g) 0 0 131 SO_3(g) -395.7 -371.1 256.3 H(g) 217 203 115 H_S(g) -20.17 -33.0 205.6 H^*(aq) 0 0 0 0 0 0 0 0 OH ⁻ (aq) -230 -157 -11 Titanium -2017 -33.0 205.6 H_2O(l) -286 -237 70 TiCl_4(g) -763 -727 355 H_O(g) -242 -229 189 TiO_(s) -945 -890 50	HF(q)	-271	-273	174	S(rhombic)	0	0	31.8
Hydrogen SO,(g) -296.8 -300.2 248.8 $H_2(g)$ 0 0 131 $SO_3(g)$ -395.7 -371.1 256.3 $H_2(g)$ 0 0 131 $SO_3(g)$ -395.7 -371.1 256.3 $H(g)$ 217 203 115 $H_5S(g)$ -20.17 -33.0 205.6 $H^+(aq)$ 0 0 0 0 0 0 0 $OH^-(aq)$ -230 -157 -11 Titanium -763 -727 355 $H_2O(l)$ -286 -237 70 TiCl_4(g) -763 -727 355 $H_2O(g)$ -242 -229 189 TiO_3(g) -945 -890 50		-/-			S(monocl)	0.3	0.1	32.6
H_2(g) 0 0 131 SO ₃ (g) -395.7 -371.1 256.3 H(g) 217 203 115 H ₂ S(g) -20.17 -33.0 205.6 H*(aq) 0 0 0 0 0 0 0 OH*(aq) -230 -157 -11 Titanium -763 -727 355 H ₂ O(l) -286 -237 70 TiCl ₄ (g) -763 -727 355 H ₂ O(g) -242 -229 189 TiO_3 -945 -890 50	Hvdrogen	1	1		$SO_{1}(\sigma)$	-296.8	-300.2	248.8
$H(g)$ 217 203 115 $H_{,S}(g)$ -20.17 -33.0 205.6 $H^*(aq)$ 0 0 0 0 0 0 $OH^-(aq)$ -230 -157 -11 Titanium $H_2O(l)$ -286 -237 70 $TiCl_4(g)$ -763 -727 355 $H_{,O}(g)$ -242 -229 189 $TiO_{,0}(c)$ -945 -890 50	Η.(σ)	0	0	131	$SO_{1}(q)$	-395.7	-371.1	256.3
H*(aq) 0 0 0 110	$H(\sigma)$	217	203	115	$H_S(q)$	-20.17	_33.0	205.6
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$H^+(aa)$	0	0	0		20.17	55.0	200.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$OH^{-}(aa)$	-230	-157	_11	Titanium	1		
$\frac{1}{H_{0}(g)} = -\frac{-242}{-242} = -\frac{229}{-242} = \frac{189}{-160} = \frac{1}{10} \frac{1}{(g)} = \frac{1}{-945} = -\frac{945}{-890} = \frac{50}{50}$	H.O(l)	-286	-237	70	$TiCl_{(q)}$	-763	-727	355
	$H_0(q)$		229	189 _	TiO.(s)	945	_890_	50

SPONTANEITY AND FREE ENERGY

Name

1. Summarize the signs (+ or –) of ΔH°_{rxn} and ΔS_{rxn} -for each of the following reactions (refer to the previous activities).

 $\Delta H^{o}_{_{rxn}} \quad \Delta S^{o}_{_{rxn}} \quad \Delta G^{o}_{_{rxn}}$

- a. $H_2O(l) \rightarrow H_2O(g)$ @25 °C
- b. $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$
- c. $Ba(OH)_2 \bullet 8H_2O(s) + 2NH_4Cl(s) \rightarrow BaCl_2(aq) + 10H_2O(l) + 2NH_3(aq)$

d.
$$H_2(g) + \frac{1}{2}O_2(g) \to H_2O(l) \text{ or } (g)$$

e. $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$

f.
$$\operatorname{Al}(s) + \frac{3}{2}\operatorname{Br}_2(l) \to \operatorname{AlBr}_3(s)$$

- 2. Circle which driving forces account for the spontaneity of each of the previous reactions.
- 3. In which reactions do the driving forces oppose each other?



Section

4. The net driving force for a chemical reaction is called the free energy (ΔG°) for the reaction. It is the energy that is free to drive the reaction rather than oppose another driving force. It can be calculated from free energies of formation (ΔG°_{f}) in the same way as enthalpies of formation. Calculate ΔG°_{rxn} for the reactions in question 1.

5. Another way to calculate the free energy is to combine the two driving forces of enthalpy and entropy to recognize the contribution of each and to compensate for any way they oppose each other. The equation for doing this (called the Gibbs free energy equation) is: $\Delta G^{\circ} = \Delta H^{\circ} - T\Delta S^{\circ}$. Calculate the free energy of the equations in question 1 using this equation, and compare your results with the values you determined from free energies of formation.

6. Use your data from question 1 to complete the blank cells for ΔG°_{rxn} when the driving forces drive in the same direction. What does the sign for ΔG°_{rxn} signify for the spontaneity of the reaction?

Sign of ∆H° _{rxn} (25 °C)	Sign of ∆S° _{rxn} (25 °C)	Sign of ∆G° _{rxn} (25 °C)	Sign of ∆G° _{rxn} at high temperature	Sign of ∆G° _{rxn} at low temperature
_	+			
+	_			
_	_			
+	+			

- 7. How does ΔG° change with increasing temperature for each of the following reactions?
 - a. $\operatorname{Al}(s) + \frac{3}{2}\operatorname{Br}_2(l) \to \operatorname{AlBr}_3(s)$
 - b. $N_2O_4(g) \rightarrow 2NO_2(g)$
 - c. $\operatorname{CO}_2(g) + 2\operatorname{H}_2\operatorname{O}(l) \rightarrow \operatorname{CH}_4(g) + 2\operatorname{O}_2(g)$
- 8. Use the Gibbs free energy equation to predict how the sign of ΔG° changes with temperature. Complete the cells in the previous table.

9. Calculate the temperature at which ΔG° is zero for the reaction.

 $\mathrm{HCl}(g)$ + $\mathrm{NH}_{3}(g) \rightarrow \mathrm{NH}_{4}\mathrm{Cl}(s)$
FREE ENERGY AND THE EQUILIBRIUM CONSTANT

Name

Section

1. The free energy drives a chemical reaction towards equilibrium. For the chemical reaction under standard conditions:

 $\begin{array}{ccc} A &+ & B \rightleftharpoons C &+ & D \\ 1 & M & 1 & M & 1 & M \end{array} \qquad Q_{c} = [C] [D] / [A] [B] \end{array}$

there are three possible values for free energy:

 $\Delta G^{\circ} < 0$ $\Delta G^{\circ} > 0$ $\Delta G^{\circ} = 0$

For each value, indicate the direction the driving force will push the reaction (right, left) and the range of values for the equilibrium constant (>1, <1, =1).

2. Values for ΔG° and K were obtained for four reactions:

K	$\Delta \mathbf{G}^{\circ}$
$1.4 imes 10^{-3}$	16,270 J/mol
$6.3 imes 10^{-5}$	23,950 J/mol
2.5×10^{-9}	49,050 J/mol
$2.4 imes 10^{-12}$	66,260 J/mol

Plot these values in ExcelTM and obtain the curve fitting equation (Hint: the proportionality constant consists of the temperature {in K} and R {in J/mol K}).

- 3. Determine ΔG° for the reaction, $N_2O_4(g) \rightarrow 2NO_2(g)$
 - a. Calculate K for the reaction at 25 °C.

b. Calculate ΔG for the reaction if the partial pressure of NO₂ is 0.1 atm and the partial pressure of N₂O₄ is 1 atm. ($\Delta G = \Delta G^{\circ} + RT \ln Q$)

INTRODUCTION TO OXIDATION REDUCTION

Name

Section

1. a. Identify each of the chemical equations below as to the reaction type (combustion, formation, or decomposition).

Chemical Equation Reaction Type $S(s) + O_2(g) \rightarrow SO_2(g)$ $2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$ $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$ $2HgO(s) \rightarrow 2Hg(l) + O_2(g)$

- b. Identify two characteristics common to these equations.
- c. Explain the historic interpretation of oxidation and reduction in chemical reactions.
- d. Define the terms oxidation, reduction, oxidizing agent and reducing agent.

2. Summarize the steps required to balance an oxidation-reduction reaction in aqueous solution.

3. a. Balance the following oxidation-reduction equation

 $H_{2}S(aq) + HNO_{3}(aq) \rightarrow S(s) + NO(g)$ (acidic solution)

b. Balance the following oxidation-reduction equation

 $\operatorname{BrO}_3^{-}(aq) + \operatorname{Fe}^{2+}(aq) \to \operatorname{Br}^{-}(aq) + \operatorname{Fe}^{3+}(aq)$ (basic solution)

c. Balance the following oxidation-reduction equation

 $\mathrm{K}_2\mathrm{S}_5(s) + \mathrm{HCl}(g) \to \mathrm{H}_2\mathrm{S}(g) + \mathrm{S}(s) + \mathrm{KCl}(s) \text{ (acidic solution)}$

GALVANIC CELLS

Name

Section

1. Go to http://introchem.chem.okstate.edu/DCICLA/voltaicCell20.html.[†] Selecting each tab in order, for the right-hand beaker select the metal Zn and the solution $Zn(NO_3)_2$. For the left beaker, select the metal Cu and the solution $Cu(NO_3)_2$. Click the On/Off switch on the voltmeter, note the cell voltage and observe the changes that occur in the electrochemical cell. In the figure below, identify the important components of the cell, i.e., the anode and cathode electrodes, the ions in solution in the anode and cathode compartments, and the salt bridge. In addition, indicate the direction of flow of electrons in the wire, and the direction of flow of ions in the salt bridge, the anode and the cathode compartments.



2. Based on the observed changes in the electrochemical cell, describe the reaction that is occurring at the surface of the anode electrode and the cathode electrode.

⁺ If you do not have access to this DCI website, your instructor will provide you with the data you will need.

3. Explain why the cations in the salt bridge migrate towards the cathode compartment and why the anions in the salt bridge migrate towards the anode compartment.

- 4. Write the oxidation-reduction equation and sketch the electrochemical cell using the following electrochemical cell notation.
 - i. $Zn(s) |Zn^{2+}(aq)| |H+(aq)| |H_2(g)| Pt (s)$

- 5. Write the oxidation-reduction equation and sketch the electrochemical cell using the following electrochemical cell notation.
 - i. $\operatorname{Cr}(s) \left| \operatorname{Cr}^{3_{+}}(aq) \right| \left| \operatorname{MnO}_{4}^{-}(aq), \operatorname{H}^{+}(aq), \operatorname{Mn}^{2_{+}}(aq) \right| \operatorname{Pt}(s)$

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EMF FOR GALVANIC CELLS

Name

Section

a. What was the cell potential (in units of volts) for the reaction between zinc metal and copper (II) nitrate? (The cell potential was measured in the previous DCI on Galvanic Cells.)[†]

 $\operatorname{Zn}(s) + \operatorname{Cu}(\operatorname{NO}_3)_2(aq) \rightarrow \operatorname{Cu}(s) + \operatorname{Zn}(\operatorname{NO}_3)_2(aq)$

b. What was the cell potential (in units of volts) for the reaction between zinc metal and hydrochloric acid?

 $Zn(s) + 2HCl(aq) \rightarrow H_{2}(g) + ZnCl_{2}(aq)$

c. What was the cell potential (in units of volts) for the reaction between zinc metal and silver (I) nitrate?

 $\operatorname{Zn}(s) + 2\operatorname{AgNO}_{3}(aq) \rightarrow 2\operatorname{Ag}(s) + \operatorname{Zn}(\operatorname{NO}_{3}),(aq)$

- 2. a. Explain the term *electromotive force* and the unit *volt*.
 - b. How is the emf in an electrochemical cell measured?

 $^{^{\}scriptscriptstyle \dagger}$ If you do not have access to this DCI website, your instructor will provide you with the data you will need.

- c. Explain the term standard emf and explain the importance of a reference half-reaction. Write the equation for the reference half-reaction and its emf.
- d. Based on the reference hydrogen electrode, determine the standard reduction potential for $Zn^{2+}(aq)$.
- e. Based on the reference hydrogen electrode, determine the standard reduction potential for $Ag^{*}(aq)$.
- f. Write the reaction between silver (I) nitrate and hydrochloric acid and calculate the emf for the reaction. Check the reaction using the simulation.
- 3. Using the table of Standard Reduction Potentials which follows, identify:
 - a. the substance most likely to be oxidized
 - b. the substance most likely to be reduced
 - c. the strongest oxidizing agent
 - d. the strongest reducing agent

- 4. Using the table of Standard Reduction Potentials on the next page, complete the following problems:
 - a. Which of the following species is the strongest oxidizing agent, MnO_4^- (in acidic solution), $Br_2(l)$, or $Ca^{2+}(aq)$?
 - b. Will aluminum displace Cu²⁺ion from an aqueous solution of Cu(NO₃)₂?
 - c. Will Mg displace Sn²⁺ from an aqueous solution of tin (II) nitrate?
 - d. Will lead metal dissolve in 1 M HCl?
 - e. From the following information estimate the E° for

$$M^{2+}(aq) + 2e^{-} \rightarrow M(s)$$

The metal, M, dissolves in 1 M HNO₃ but not in 1 M HCl. It will displace $Ag^{+}(aq)$, but not $Cu^{2+}(aq)$.

Standard Reduction Potentials at 25°C					
Ha	lf–Re	action	E°		
$F_2(g) + 2e^-$	\rightarrow	2F-(<i>aq</i>)	+2.87 v		
$H_2O_2(aq) + 2H^+(aq) + 2e^-$	\rightarrow	2H ₂ O(<i>l</i>)	+1.77 v		
$MnO_{4}^{-}(aq) + 8H^{+}(aq) + 5e^{-}$	\rightarrow	$Mn^{2+}(aq) + 4H_2O(l)$	+1.52 v		
$Au^{3+}(aq) + 3e^{-}$	\rightarrow	Au(s)	+1.50 v		
$\operatorname{Cl}_2(g) + 2e^-$	\rightarrow	$2\mathrm{Cl}^{-}(aq)$	+1.36 v		
$Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^-$	\rightarrow	$2Cr^{3+}(aq) + 7H_2O(l)$	+1.33 v		
$O_2(g) + 4H^+(aq) + 4e^-$	\rightarrow	2H ₂ O(<i>l</i>)	+1.23 v		
$\operatorname{Br}_2(l) + 2e^{-l}$	\rightarrow	2Br ⁻ (<i>aq</i>)	+1.07 v		
$NO_{3}^{-}(aq) + 4H^{+}(aq) + 3e^{-}$	\rightarrow	$NO(g) + 2H_2O(l)$	+0.96 v		
$Ag^+(aq) + 1e^-$	\rightarrow	Ag(s)	+0.80 v		
$I_2(s) + 2e^{-1}$	\rightarrow	$2I^{-}(aq)$	+0.53 v		
$O_2(g) + 2H_2O(l) + 4e^{-1}$	\rightarrow	4OH-(<i>aq</i>)	*0.40 v		
$\mathrm{Cu}^{2+}(aq) + 2\mathrm{e}^{-}$	\rightarrow	Cu(s)	+0.34 v		
$\operatorname{AgCl}(s) + 1e^{-}$	\rightarrow	$Ag(s) + Cl^{-}(aq)$	+0.22 v		
$2\mathrm{H}^+(aq) + 2\mathrm{e}^-$	\rightarrow	H ₂ (s)	0.00 v		
$Pb^{2+}(aq) + 2e^{-}$	\rightarrow	Pb(s)	-0.13 v		
$\operatorname{Sn}^{2+}(aq) + 2e^{-}$	\rightarrow	Sn(s)	-0.136 v		
$Ni^{2+}(aq) + 2e^{-}$	\rightarrow	Ni(s)	-0.25 v		
$\mathrm{Co}^{2+}(aq) + 2\mathrm{e}^{-}$	\rightarrow	Co(s)	-0.28 v		
$\mathrm{Fe}^{2+}(aq)+2\mathrm{e}^{-}$	\rightarrow	Fe(s)	-0.44 v		
$\operatorname{Zn}^{2+}(aq) + 2e^{-}$	\rightarrow	Zn(s)	–0.76 v		
$2H_2O(l) + 2e^{-l}$	\rightarrow	$\mathrm{H_2}(g) + 2\mathrm{OH}^{-}(aq)$	-0.83 v		
$\operatorname{Cr}^{2+}(aq) + 2e^{-}$	\rightarrow	Cr(s)	-0.91 v		
$Mn^{2+}(aq) + 2e^{-}$	\rightarrow	Mn(s)	-1.18 v		
$Al^{3+}(aq) + 3e^{-}$	\rightarrow	Al(s)	-1.66 v		
$Mg^{2+}(aq) + 2e^{-}$	\rightarrow	Mg(s)	-2.37 v		
$Na^+(aq) + 1e^-$	\rightarrow	Na(s)	-2.71 v		
$Ca^{2+}(aq) + 2e^{-}$	\rightarrow	Ca(s)	-2.87 v		
$Ba^{2+}(aq) + 2e^{-}$	\rightarrow	Ba(s)	-2.90 v		
$K^{+}(aq) + 1e^{-}$	\rightarrow	K(s)	-2.93 v		
$\text{Li}^+(aq) + 1e^-$	\rightarrow	Li(s)	-3.05 v		

NERNST EQUATION

Section

1. During the reaction between zinc metal and copper (II) nitrate the measured cell potential changes. In the table below the measured cell potential, E_{cell} is shown as the concentration of $Zn^{2+}(aq)$ and $Cu^{2+}(aq)$ change.

Experiment	E _{cell}	E°	[Zn ²⁺]	[Cu ²⁺]
1	0.760	0.76	1	1
2	0.757	0.76	1.1	0.9
3	0.755	0.76	1.2	0.8
4	0.752	0.76	1.3	0.7
5	0.749	0.76	1.4	0.6
6	0.746	0.76	1.5	0.5
7	0.742	0.76	1.6	0.4
8	0.738	0.76	1.7	0.3
9	0.732	0.76	1.8	0.2
10	0.722	0.76	1.9	0.1
11	0.692	0.76	1.99	0.01

a. How does the cell potential change during the reaction?

Name

b. When the data is plotted E_{cell} versus $log\left(\frac{[Zn^{2+}]}{[Cu^{2+}]}\right)$ a straight line with a negative slope is obtained (try it yourself). Careful consideration of this reaction and other reactions yields the following relationship between the cell potential and concentration of reactants and products.

$$\mathbf{E}_{\text{cell}} = \mathbf{E}^{\circ} - \frac{0.0591}{n} \quad \log\left(\frac{\left\lfloor \mathbf{Z}n^{2+} \right\rfloor}{\left\lceil \mathbf{C}u^{2+} \right\rceil}\right)$$

where n is the number of electrons transferred in the balanced oxidation-reduction reaction and the concentration of products divided by reactants. You should recognize the ratio of concentration as Q for the reaction. Try one of the Experiments to see that you can calculate the E_{cell} for the reaction.

- 2. Complete the following problems:
 - a. Calculate E° for the reaction

$$\operatorname{Zn}(s) + \operatorname{Cu}^{2+}(aq) \to \operatorname{Zn}^{2+}(aq) + \operatorname{Cu}(s)$$

- i. Calculate E_{cell} when the ratio of these concentrations is small, that is, if $[Zn^{2+}] = 1 \times 10^{-4} M$ and $[Cu^{2+}] = 1.0 M$.
- ii. Calculate E_{cell} when the ratio of these concentrations is large, that is, if $[Cu^{2+}] = 1 \times 10^{-4} \text{ M}$ and $[Zn^{2+}] = 1.0 \text{ M}$.
- b. Which of the following oxidizing agents become stronger as the [H⁺] is increased? Which are unchanged? Which become weaker?
 - i. Br₂
 - ii. Fe³⁺
 - iii. MnO₄-
 - iv. H⁺
 - v. $Cr_2O_7^{2-}$
- c. Calculate E_{cell} for:

 $Cu(s) \|Cu^{2+}(aq) (3.00 \text{ M})\|Cu^{2+}(aq) (0.100 \text{ M})\|Cu(s)\|$

BATTERIES

Section

Name

1. a. Write the chemical equation which describes the discharge reaction in an alkaline dry cell battery used in flashlights or transistor radios.



- b. Write the chemical equation which describes the discharge reaction in a lead-acid battery used in automobiles.
- 2. a. Write the chemical equations involved in the corrosion of iron.

b. Sketch a simple diagram showing the location of the two half–reactions involved in the corrosion of iron.

3. Distinguish between a voltaic cell and an electrolytic cell.

ELECTROLYSIS I

Name

Section

1. a. Write the chemical equation for the industrial preparation of $Cl_2(g)$ in the absence of water.

b. Write the chemical equation that describes the reaction that occurs when NaCl is electrolyzed in water.

c. Explain why different products are formed in the electrolysis of NaCl(*l*) and NaCl(*aq*).

- d. Predict the products when the following solutions are electrolyzed between inert electrodes.
 - i. $Na_2SO_4(aq)$

ii. CuSO₄(*aq*)

iii. KI(l)

ELECTROLYSIS II

Name

Section

- 1. When one amp of electricity passes through an electrical circuit for one second, the equivalent of one coulomb of charge passes through the circuit. If the charge on a single electron is 1.60×10^{-19} coulombs how many electrons must pass a point to transfer 1 coulomb of charge?
- 2. If this number of electrons pass the point in one second, then 1 coulomb of charge is transferred. This is an amp. The ampere is the time rate of change of electrical charge.
- 3. How many coulombs of charge passes through an electrical circuit when 5.5 amps of current flow for 10 seconds? For 60 seconds? For 30.0 minutes?
- 4. If the charge on a single electron is 1.60×10^{-19} coulombs, how many electrons have flowed through the circuit when 5.5 amps of current flows for 10 seconds? For 60 seconds? For 30.0 minutes?
- 5. How many mol of electrons have flowed through the circuit when 5.5 amps of current flows for 10 seconds? For 60 seconds? For 30.0 minutes?
- 6. If the charge on a single electron is 1.60×10^{-19} coulombs, what is the total charge that must pass through the circuit when 1.00 mol of electrons pass through an electrical circuit?

7. When water is electrolyzed, hydrogen and oxygen gas are formed according to the reaction,

$$2H_2O(l) \rightleftharpoons 2H_2(g) + O_2(g)$$

- a. Write the two half-reactions for the electrolysis of water.
- b. How many mol of electrons are required to produce 2 mol of H,?
- c. How many mol of electrons are required to produce 1 mol of O₂?
- 8. Using the information above, complete the following table.

Time of current flow in minutes	Time of current flow in seconds	Current (amperes)	Number of Coulombs that flow	Number of mol of electrons that flow	Half-reaction	Mass of gas/metal produced (grams)
10	600	5.5	3300	3.42 × 10 ⁻²	$2e^{-} + 2H_2O \rightarrow$ $2H_2(g) + 2OH^{-}$	6.84 × 10 ⁻²
10	600	5.5	3300	3.42 × 10 ⁻²	$2H_2O \rightarrow O_2(g) + 4H^+ + 4e^-$	2.74 × 10 ⁻¹
25		5.5			$2e^{-} + 2H_2O \rightarrow$ $2H_2(g) + 2OH^{-}$	
25		5.5			$2H_2O \rightarrow O_2(g) + 4H^+ + 4e^-$	
15		6.0			$e^- + Ag^+(aq) \rightarrow Ag(s)$	
		7.2	42,000		$2e^- + Cu^{+2}(aq)$ $\rightarrow Cu(s)$	
7.5					$2e^- + Cu^{+2}(aq)$ $\rightarrow Cu(s)$	8.25 g

- 9. Complete the following problems:
 - a. What weight of cadmium will be deposited from a $CdCl_2$ solution by passage of a current of 1.50 amps for 30.0 minutes?

- b. Consider an electrolysis that results in the production of 1.00 g of Cu metal from CuSO₄.
 - i. How many coulombs of electricity are required?

ii. If the reduction takes 1 hour, how many amps are required?

Computer Lab Activities



MoLEs

Introduction to MoLEs Activities Kinetics

- Mechanisms of a Chemical Reaction
- Speeds of a Chemical Reaction
- Rates of a Chemical Reaction
- Catalysts
- Activation Energy
- Kinetic Systems and Research Statements Equilibrium
 - Shifting Reactions A
 - Shifting Reactions B
 - Extent of a Chemical Reaction
 - Equilibrium Systems and Research Statements

Acid/Base Chemistry

- Acid/Base Classifications
- Acid/Base Interactions

Laboratory Simulations

Introduction to Laboratory Simulations Kinetics

- Iodine Clock
- Concentration/Temperature Effects
- Decomposition of H₂O₂

Acid/Base

- Acid/Base pH
- Acid/Base Titrations
- Acid/Base Salts
- Buffers

Electrochemistry

- Activities of Metals
- Voltaic Cells
- Concentration Cells
- Electrolysis
- Acid/Base Systems and Research StatementsT FOR DISTRIBUTION - FOR INSTRUCTORS USE ONLY

NOT FOR DISTRIBUTION - FOR INSTRUCTORS USE ONLY

MoLEs



Introduction to MoLEs Activities—Computer Simulations*

Molecular Level Experiments (MoLEs) are chemistry laboratory experiments based on computer simulations. There are two types of simulation programs that can be used in these activities: Particulate Simulations and Graphic Simulations.

To begin an activity you must be able to log on to the Internet using Internet Explorer (Microsoft) 4.5 or higher or Safari with OSX for Macs.

* Michael R. Abraham & John Gelder, September 2002. Project supported by NSF-CCLI-EMD #0127563 🗱

Particulate Simulations

Once the browser is running, type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/Sample.htm

This should load a sample Particulate Simulation. Once you have the simulation running, your screen should look similar to what is shown in Figure 1 below.





Although the details of the screen you will see will vary with different MoLE activities, all Particulate Simulations have three important regions. The Sample Region has the most activity. It is a container with different kinds of particles. To explore the behavior of the sample you can change the variables located in the Control Bar Region. The Control Bar Region has scrollbars that allow you to change the variables of the experiment. There are scrollbars for pressure (in units of atmospheres), for volume (in units of liters), for the amounts of each substance that is active in the Sample Region (in mols), and for temperature (in units of Kelvins). The concentration of each substance can be calculated by dividing the number of mols by the volume of the container. To the left of each scrollbar is a radio button. When selected, that particular variable (called the dependent variable) is calculated based on the value of the other variables. In the default mode the pressure scrollbar's radio button is selected so the pressure of the sample is varied. As a simple exploration, try moving each of the scrollbars and observe the effect on the sample. These effects will be addressed in more detail in each experiment. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions. The Pause button will suspend the motion in the gas sample while the Enable Tracking button will turn the red tracking line on and off.

The region below the Control Bar Region is the Module Display Region. This region allows the data in the other regions to be represented graphically or in tables in several ways depending on the particular activity you are doing. These might include simple graphs comparing variables, concentration strip charts showing concentrations vs. time, energy reaction profiles showing the relative energies of reactants and products of a chemical reaction, and a replay feature that allows you to replay and slow down a portion of the particulate interactions showing in the Sample Region. To utilize these different functions use the pull-down menu located below the temperature scrollbar.

The Concentrations option shows the relative concentrations and changes in concentration vs. time for each substance studied in the simulation. Manipulate the concentrations using the Control Bars to see how the strip chart is affected. These effects will be addressed in more detail in experiments that utilize this function. You can click on the Reset button located below the temperature scrollbar to return to the original conditions.

The Replay option (see Figure 2) allows you to slow down the motion in the Sample Region and to replay portions of the reaction sequence. You can click on the Pause Button and, using the forward or reverse arrows on the time index function, view the motion of the particles a step at a time. These effects will be addressed in more detail in experiments that utilize this function. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions.

Replay		*
(0+	time index30.00



The Kinetics option allows you to record quantitative information being generated by the strip chart. Three columns of data are generated: time, amount, and instantaneous rate. These data are generated by specifying the compound you want to follow and then clicking on the Get Data button. This can be done as many times during the reaction as you want. These effects will be addressed in more detail in experiments that utilize this function.

The Reaction Viewer shows the reaction profile for a chemical reaction as it proceeds from reactants to products. These effects will be addressed in more detail in experiments that utilize this function.

The Relations option reveals an xy graph with a dropdown menu on each axis. Selecting the dropdown menu on either axis provides a list of the variables shown in the Control Bar Region. The two buttons, Enable and Multiple, are used when plotting pairs of variables. If you select pressure for the y-axis and volume for the x-axis, and then select "Enable," these same variables are activated in the Control Bar Region. By scrolling the volume slide bar in the Control Bar Region, you will trace out a plot. The Multiple Button allows two or more plots to be superimposed.

The Velocities option is a plot of the speed distribution of the sample. The y-axis of this plot represents the number of particles. The x-axis represents the range of velocities starting at zero. The bars in this plot represent the velocities of the particles in the Sample Region. As the velocities of the particles change, the plot is redrawn. The smooth curved line in the plot represents the ideal distribution of the velocities for the gas sample. A vertical line represents the average (root-mean-square average) speed of the sample. This line is the same color as the particles. Observe the behavior of this region while changing each of the variables in the Control Bar Region. If you click on the Enable Tracking button, you can follow the path of a particle in the Sample Region. The length of the tail represents a fixed unit of time, and consequently can be used as a measure of the speed of the particle. This same particle is identified as a red line, labeled with the actual speed (in meters/second), in the speed distribution plot. If you pause the motion of the particles, you can click on different particles to get a measure of their speeds.

If you have any questions, check with another student in the class, or your instructor.

Graphic Simulations

Once the browser is running, type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/SampleG.htm

This should load a sample Graphic Simulation. Once you have the simulation running, your screen should look similar to what is shown in Figure 3. Although the details of the screen you will see will vary with different MoLE activities, all Graphic Simulations have three important regions. The Strip Chart Region will plot the relative concentrations versus time of all the substances in the reaction to be studied. When you first load the program, the Strip Chart Region is blank. It is activated when you click on the Resume button.



Figure 3.

The Control Bar Region has scrollbars that allow you to change the variables of the experiment. There are scrollbars for pressure (in units of atmospheres), for volume (in units of liters), for the amounts of each substance that is active in the Sample Region (in mols), and for temperature (in units of Kelvins). The concentration of each substance can be calculated by dividing the number of mols by the volume of the container. To the left of each scrollbar is a radio button. When selected, that particular variable (called the dependent variable) is calculated based on the value of the other variables. In the default mode the pressure scrollbar's radio button is selected so the pressure of the sample is varied.

As a simple exploration, try moving each of the scrollbars and observe the effect on the strip chart. These effects will be addressed in more detail in each experiment. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions. The Pause button will suspend the motion in the gas sample.

The region below the Control Bar Region is the Module Display Region. As was the case for the Particulate Simulation this region allows the data in the other regions to be represented in several ways depending on the particular activity you are doing. These might include energy reaction profiles showing the relative energies of reactants and products of a chemical reaction, and simple graphs comparing variables. To utilize these different functions, use the pull-down menu located below the temperature scrollbar.

The Kinetics option allows you to record quantitative information being generated by the strip chart. Three columns of data are generated: time, amount, and instantaneous rate. These data are generated by specifying the compound you want to follow and then clicking on the Get Data button. This can be done as many times during the reaction as you want. These effects will be addressed in more detail in experiments that utilize this function.

The Reaction Viewer shows the reaction profile for a chemical reaction as it proceeds from reactants to products. These effects will be addressed in more detail in experiments that utilize this function.

The Relations option reveals an xy graph with a dropdown menu on each axis. Selecting the dropdown menu on either axis provides a list of the variables shown in the Control Bar Region. The two buttons, Enable and Multiple, are used when plotting pairs of variables. If you select pressure for the y-axis and volume for the x-axis, and then select "Enable," these same variables are activated in the Control Bar Region. By scrolling the volume slide bar in the Control Bar Region, you will trace out a plot. The Multiple Button allows two or more plots to be superimposed.

If you have any questions, check with another student in the class, or your instructor.

MECHANISMS OF A CHEMICAL REACTION

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/KRGBM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: How does a chemical reaction proceed from reactants to products?

I. Data Collection

Open the molecular simulation KRGBM:

http://introchem.chem.okstate.edu/DCICLA/KRGBM.htm

A. Based on what you observe in the sample region and control bar region of the screen, record the number and the concentration of R, BG, B, and RG particles in the table below.

	R	BG	В	RG
# of Particles				
Concentration (M)				

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Record your observations of what is happening. Use some or all of the following terms in your description: atom, molecule, particle, collision, effective collision, speed, energy, orientation, reactants, and products.

C. Allow the simulation to run until no more changes occur. Click on the Pause button and record your observations. Record the number and concentration of each kind of particle.

	R	BG	В	RG
# of Particles				
Concentration (M)				

II. Data Analysis and Interpretation

A. Write a balanced equation for the reaction you have observed in this simulation. (Simplify the equation so that no common particles are on both sides of the equation and it represents the lowest ratio of whole numbers of particles.)

B. Draw and label the appearance of the strip chart. Identify each kind of particle on the strip chart and explain what is happening to each over time.

C. What criteria did you use to decide the reaction was finished?

III. Data Collection

Reset the simulation. Then click on the Resume and Enable Reactions buttons. Systematically observe multiple collisions between each of the possible combinations of pairs of the reactant and product particles (see the table below). Note when pairs of collisions result in a change. Use the following table to guide and record your observations. In order to aid your observations you can do the following: (a) change the amounts of the reactant and product particles, (b) use the Enable Tracking button with different particles, (c) use the replay option, (d) change the volume of the container, and (e) change the temperature of the sample.

Collisions Between					
Particle 1	Particle 2	Result	Speed	Orientation	Comments
R	R	No reaction			
R	BG				
R	В				
R	RG				
BG	В				
BG	BG				
BG	RG				
В	В				
В	RG				
RG	RG				

IV. Data Analysis and Interpretation

A. Use the data from the table to write a balanced equation to represent your observations. Compare this equation with the one you wrote for section II.A.

B. Even those collisions between particles that can result in a change don't do so 100% of the time. From your observations can you propose at least two different reasons why some collisions result in a change and others don't.

V. Conclusions

In the boxes below, draw pictures showing how a possible collision between reactant molecules might form product molecules for the KRGBM reaction. Make sure the orientation of the collision supports the arrangement of the atoms in the reactant and product molecules.



VI. Data Collection

Open the molecular simulation K2GBM:

http://introchem.chem.okstate.edu/DCICLA/K2GBM.htm

A. Based on what you observe in the sample region and control bar region of the screen, record the number and the concentration of the particles in the table below.

	G	В	G ₂	GB	G ₂ B	B ₂
# of Particles						
Concentration (M)						

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Record your observations of what is happening.

C. Allow the simulation to run until no more changes occur. Click on the Pause button and record your observations. Record the number and concentration of each kind of particle.

	G	В	G ₂	GB	G ₂ B	B ₂
# of Particles						
Concentration (M)						

VII. Data Analysis and Interpretation

A. Write an overall balanced equation to represent your observations.

B. Draw and label the appearance of the strip chart. Identify each kind of particle on the strip chart and label what is happening to the particles at each change in the chart.

C. What criteria did you use to decide the reaction was finished?

VIII. Data Collection

A. Use the simulation to design and carry out experiments to explore all of the possible collisions between reactant particles. In order to aid your observations you can do the following: (a) change the amounts of the reactant and product particles, (b) use the Enable Tracking button with different particles, (c) use the replay option, (d) change the volume of the container, and (e) change the temperature of the sample. Use the following table to guide and record your observations.

Reactant 1	Reactant 2	Result	Comments
В	В		
В	G		
G	G		

Describe the experiments you carried out.

Write the chemical equation(s) to summarize the experiments.

B. In a manner similar to section VIII.A., design and carry out additional experiments to explore further all of the possible collisions between the product molecule(s) you identified from section VII.A. with the other reactant particles. Design and construct a table to record your observations.

Describe the experiments you carried out.
Write the chemical equation(s) to summarize the experiments.

IX. Conclusions

A. Using the data you collected in part VIII, propose a step-by-step process (mechanism) showing how the reaction in the molecular simulation K2GBM proceeds from reactants to final products.

B. An alternate possible mechanism that has been proposed for the reaction in the molecular simulation K2GBM is a one-step process described by the following: $2G + B \rightarrow G_2B$. Why is this mechanism less likely than the one you observed?

SPEEDS OF A CHEMICAL REACTION

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/K2RM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.





Problem Statement: What factors influence how fast a chemical reaction proceeds?

I. Data Collection

Open the molecular simulation K2RM:

http://introchem.chem.okstate.edu/DCICLA/K2RM.htm

A. Record what you observe in the sample region of the screen. Indicate the number and the concentration of the reaction particles.

	R	R ₂
# of Particles		
Concentration (M)		

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run until no more changes occur. Click on the Pause button and record the number and the concentration of the reaction particles.

	R	R ₂
# of Particles		
Concentration (M)		

C. Reset the simulation. Calibrate the time axis (x-axis) of the Concentration Strip Chart. To do this, click on the Resume button and with a stopwatch time how long it takes for the strip chart line to proceed across the graphing space. Measure the length of the line in millimeters (mm) with a ruler. Record your data in the spaces below. Develop a formula for converting mm to seconds.

Time (in sec)	
Time (in mm)	
Formula	1 mm = seconds

D. Click on the Reset button. Determine and record the initial concentration of R ([R]_i in units of mols/L). Record the temperature of the sample. Click on the Enable Reactions button and then click on the Resume button. Pause the reaction when five product particles are formed and measure the time elapsed by measuring the time on the strip chart's x-axis using the length (in mm) as a measure of time. Determine and record the final concentration ([R]_p). Repeat this experiment two more times and record your results in the following table. Calculate the average time.

	Trial 1	Trial 2	Trial 3	Average
Temperature				
Time (mm)				
Time (sec)				

E. Repeat the procedure in section I. D. at a temperature of 400K. (When resetting for a new trial, don't forget to reset the temperature to 400K.)

[R]_i =_____ [R]_f = _____

	Trial 1	Trial 2	Trial 3	Average
Temperature				
Time (mm)				
Time (sec)				

F. Repeat the procedure in section I. D. with 20 moles of R.

 $[R]_i = _$ $[R]_f = _$

	Trial 1	Trial 2	Trial 3	Average
Temperature				
Time (mm)				
Time (sec)				

II. Data Analysis and Interpretation

A. Write a balanced chemical equation for the reaction you observed in this simulation. (Simplify the equation so that no common particles are on both sides of the equation and it represents the lowest ratio of whole numbers of particles.)

B. Copy the initial concentrations $([R]_i)$ and the final concentrations $([R]_i)$ from section II into the following table. Determine the change in concentration $([R]=[R]_f-[R]_i)$ of the reactant R for each of the experiments you did in sections I.D., E., and F. Use the average values in your calculations.

	I. D	I. E	I. F
[R] _i			
[R] _f			
[R]			

C. What is the sign (positive or negative) of the change in concentration? What is the meaning of the sign?

D. How is the time it takes for a reaction to proceed related to the speed of the reaction?

E. The speed for an automobile is expressed in units of miles per hour (change in distance divided by the change in time). Since what changes in a chemical reaction is not distance (see section II.D.), what units would you use for the speed of a chemical reaction?

F. Using the data from II.D., calculate the speeds for the three experimental conditions you explored in sections I.D., E., and F., using the average data you collected. Make sure you include the units for the speeds.

Speed of the reaction for conditions in section I.D. (starting with 12 mol R, temperature = 275K)

Speed of the reaction for conditions in section I.E. (starting with 12 mol R, temperature = 400K)

Speed of the reaction for conditions in section I.F. = (starting with 20 mol R, temperature = 275K)

G. Chemists refer to the speed of a chemical reaction as its rate. Write a statement summarizing the effect that temperature has on the rate of a chemical reaction. What is the evidence for your statement? Propose a reason(s) why temperature has this effect. Use a molecular explanation.

H. Write a statement summarizing how the initial concentration of the reactants influences the rate of the chemical reaction. What is the evidence for your statement? Propose a reason(s) why concentration has this effect.

RATES OF A CHEMICAL REACTION

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/KRGO1N.htm

This will load a Graphics Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: How is the rate of a chemical reaction related to the initial concentration of the reactants?

I. Data Collection

Open the graphic simulation KRGO1N:

http://introchem.chem.okstate.edu/DCICLA/KRGO1N.htm

A. Use the information there to write a balanced equation for the reaction you will be studying in this activity. Use the information in the Control Bar Region to determine the initial concentrations of the reactants and products in the reaction. Record this information in the space below.

B. Click on the Reset button. Click on the Enable Reactions and then the Resume buttons to begin the reaction. When the concentrations stop changing, click Pause to stop the action. In the space below, draw the appearance of the strip chart graph and label the axes. If necessary, use the scrollbar located under the strip chart to move the chart back to the beginning of the reaction. Identify the chemical substances that correspond to each of the colored lines. Interpret the meaning of the shape of the lines on the graph? What do these lines tell you about the rate of the reaction?

C. Click on the Reset button. In the drop-down menu in the Module Control Region select Kinetics. Record the value for the initial concentration of RG, $[RG]_0$. Click on the Enable Reactions button and then the Get Data button and record the rate at t=0, the initial rate, for this set of conditions in the table below.

Experiment #	[RG] ₀ (M)	Initial Rate (M time ⁻¹),-[RG]/time
1		

D. Click on the Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Collect some additional time and amount data for RG by repeatedly clicking on the Get Data button while the reaction is proceeding. Graph the time vs. the amount of reactant on a piece of graph paper. (The easiest way to do this is to highlight and copy the data on the screen and then paste it into a graphing program. Microsoft Excel is one possibility.) Describe the form of the graph.

E. Plot the first two data points of your graph and determine the slope of the graph (include the units for the slope). Record this value below. Show your work on the graph paper and submit it with your report. What does the slope represent? Compare this value with the initial rate of the consumption of RG in the table above.

F. Use the drop-down menu for the Compound to see the data points for the formation of G. Record the initial rate for the production of G. Graph the time vs. the amount of product on a piece of graph paper. Describe the form of the graph. Plot the first two data points of your graph and determine the slope of the graph. Show your work on the graph paper and submit it with your report. What does the slope represent? Compare this value with the initial rate of the production of G. What is the initial rate for the production of the other product, R?

II. Data Analysis and Interpretation

A. What happens to the rate of the reaction as time passes? Use both the strip chart graph and your data points as evidence for your conclusion.

B. Compare the rate of the consumption of RG with the production of G and R. How are they related? How do you account for this relationship?

C. Under what circumstances are you justified in using the slope of a straight line to determine the initial rate of a chemical reaction with the data you have collected?

III. Data Collection

In the table below record the concentration and the initial rate of the consumption of RG you measured in section I.C. Reset the simulation. Adjust the Compound setting to monitor the kinetics of the reactant RG. Change the amount of RG to 2 mols. Click on the Enable Reactions, the Get Data, and finally the Resume buttons to begin the reaction. Record the initial concentration and the initial rate of the consumption of RG for this new concentration. Collect sets of rate data for 0.25 mols of RG, 0.5 mols of RG, and 1.5 mols of RG.

Experiment #	[RG] ₀ (M)	Initial Rate (M time ⁻¹),—[RG]/time

IV. Data Analysis and Interpretation

- A. How does doubling the concentration of RG affect the rate of the reaction?
- B. Construct a mathematical relationship (called a rate law) between the rate of the reaction and the initial concentration of RG. (Hint: Write a proportionality equation based on the data you collected in section III. Determine how the concentration changes for any two trials and then what is the corresponding change in the rate.)

C. Using your data from section III., determine the value for the proportionality constant (called the rate constant, k) for the equation you generated in section IV.B. for each set of data you collected in section III.

D. Propose a reason for calculating the rate constant for your reaction. Why not just use the value of the rate?

E. Optional: Another way to express the rate law is to determine the mathematical relationship between the concentration of the reactant and the time. This form of the rate law for the reaction you are studying can be determined from the kinetics data you previously generated from the simulation. Using a graphing program, plot the amount of RG vs. the time. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line. Compare the equation of this best-fit line with the data you collected in previous sections.

F. Click on the Reset button. Click on the Enable Reactions, Get Data, and then the Resume buttons to begin the reaction. As the reaction proceeds across the Strip Chart Region window, click on the Get Data button several times to collect additional data, and then pause the reaction. There is a drop-down menu below the Strip Chart Region. The default position shows that concentration (symbolized as []) is being plotted on the y-axis against time on the x-axis. The y-axis can be changed to two other options: the natural logarithm of the concentration (symbolized as In[]), and the reciprocal of the concentration (symbolized as 1/[]). Use your observations of these three options to plan the function of the amount of RG you will graph vs. time to generate a mathematical equation for your data. Graph that function of amount vs. time and determine the equation of the line. Compare the values in the equation with the values you developed in the equations from previous sections (Sections IV.B., IV.C., and IV.E.).

G. Do you think the rate law you determined for the reaction you are studying would be the same for all reactions? Why or why not?

V. Data Collection

Open the graphic simulation K2RN:

http://introchem.chem.okstate.edu/DCICLA/K2RN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Reset the simulation. In the drop-down menu in the Module Control Region select Kinetics. Design experiments to investigate the relationship between the rate of consumption of reactant and the initial concentrations of the reactants of the reaction. (Refer to section III.) Fill in the concentrations and the name of the reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[]	Initial Rate Reactant,-[]/t
1	1.0mol/40L=0.0250M	
2	2.0mol/40L=0.0500M	
3	0.333mol/40L=0.008325M	

C. Reset the simulation. In the drop-down menu in the Module Control Region select Kinetics. Click on the Enable Reaction, Get Data, and finally the Resume buttons. As the reaction proceeds across the Strip Chart Region window, click on the Get Data button several times to collect additional data, and then pause the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes. How is this graph different from the one you sketched in section I.B.?

D. Graph the time vs. the amount of reactant on a piece of graph paper. Describe the form of the graph. Using the suggestions in section IV.F., determine the mathematical equation for the best-fit line.

VI. Data Analysis and Interpretation

- A. How does doubling the concentration of R affect the rate of the reaction?
- B. How does tripling the concentration of R affect the rate of the reaction?

C. Determine the rate law for the reaction you are studying in terms of the rate and the concentration of reactant (see section IV.B.). Determine the rate constant for the reaction (see section IV.C.).

D. What does the equation you constructed in section V.D. represent? What does the numerical amount (slope) in the equation represent?

E. Propose a mechanism to explain and describe how the reactant particles for this reaction interact to form product particles. (You can also view the mechanism with the molecular simulation of this reaction at http://introchem.chem.okstate.edu/DCICLA/K2RM.htm.)

F. How would you characterize the mechanism in terms of the number of the original reactant particles necessary for each individual reaction to occur? How is this related to the rate law you proposed?

G. Compare the rate law and conclusions concerning the number of necessary reactant particles in this section with that of the rate law and number of necessary reactant particles for the reaction in section IV.B. (You can view the mechanism of this reaction with the molecular simulation of this reaction at http://introchem.chem.okstate.edu/DCICLA/KRGO1M.htm.) How would you account for the differences in the rate laws?

VII. Data Collection

Open the graphic simulation K2GBN:

http://introchem.chem.okstate.edu/DCICLA/K2GBN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Reset the simulation. Change the Module Control Region to view the kinetics table. Adjust the compound setting drop-down menu so that you will gather data for the production of compound G₂B. Click on the Enable Reactions button, Click on the Get Data, and finally the Resume buttons. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

C. Determine the initial rate of production of the product G₂B, [G₂B]/time, for the reaction. (See section I.E.)

D. Design experiments to investigate the relationship between the rate of production of the product G_2B and the initial concentrations of the reactants of the reaction you are studying. (Refer to section III.) Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[]	[]	Initial Rate, [G ₂ B]/time

VIII. Data Analysis and Interpretation

A. What effect does doubling the concentration of G have on the initial rate of the reaction?

B. What effect does doubling the concentration of B have on the initial rate of the reaction?

C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants B and G (see section IV.B.). Determine the rate constant for the reaction.

IX. Data Collection

Return to the simulation and use the pull-down menu in the Module Control Region to expose the Reaction Viewer. Use the Reactions pull-down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. (You can also view the mechanism with the molecular simulation of this reaction at http://introchem.chem.okstate.edu/DCICLA/ K2GBM.htm.) Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

X. Data Analysis and Interpretation

A. How would you characterize each step in the mechanism in terms of the number of the original reactant particles necessary for the stoichiometry of the reaction? How is this related to the rate law you proposed in section VIII.? B. How would you characterize the number and kind of reactant particles necessary to determine the rate of the overall reaction?

C. Below is the reaction profiles for step one and step two of the mechanism of the reaction you are studying. Each profile shows how the energy of that step changes as the reaction proceeds from reactants to products. Compare the profiles with each other and use them to explain why each reactant particle is necessary or not necessary to determine the rate of the reaction.



D. Identify any particles not part of the overall reaction but that are present in the mechanism. What role do these particles play in the reaction?

CATALYSTS

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/KCatBGM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: What factors influence how fast a chemical reaction proceeds?

I. Data Collection

Open the molecular simulation KCatBGM:

http://introchem.chem.okstate.edu/DCICLA/KCatBGM.htm

A. Record what you observe in the sample region of the screen. Indicate the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run until no more changes occur. Click on the Pause button and record the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

C. Reset the simulation. Calibrate the time axis (x-axis) of the Concentration Strip Chart. To do this, click on the Resume button and with a stopwatch time how long it takes for the strip chart line to proceed across the graphing space. Measure the length of the line in millimeters (mm) with a ruler. Record your data in the spaces below. Do this two more times and calculate an average. Use the average to develop a formula for converting mm to seconds.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

Formula: 1 mm = _____ seconds

D. Click on the Reset button. Click on the Enable Reactions button and then click on the Resume button. Pause the reaction when eight product particles are formed and measure the time elapsed by measuring the time on the strip chart's x-axis using the length (in cm) as a measure of time. Repeat this experiment two more times and record your results in the following table. Calculate the average time.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

II. Data Analysis and Interpretation

A. Write a balanced equation for the reaction you observed in this simulation.

B. Determine the average rate of the reaction to produce eight product particles. Express this rate with respect to the appearance of product BG in units of [BG]/s.

III. Data Collection: Add Particle R as a Reactant

A. Reset the simulation. Add 2.000 moles of particle R to the reactants. Record what you observe in the sample region of the screen. Indicate the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run until no more changes occur. Click on the Pause button and record the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

Collisions Between					
Particle 1	Particle 2	Result	Comments		
В	G				
В	R				
G	R				
В	RB				
G	RB				

C. Study the details of this reaction by observing the interactions between the following pairs of particles.

D. Click on the Reset button. Add 2.000 moles of particle R to the reactants. Click on the Enable Reactions button and then click on the Resume button. Pause the reaction when eight product particles are formed and measure the time elapsed by measuring the time on the strip chart's x-axis using the length (in cm) as a measure of time. Repeat this experiment two more times and record your results in the following table. Don't forget to add the 2 moles of particle R each time. Calculate the average time.

	Trial 1	Trial 2	Trial 3	Average
Time (in mm)				
Time (in sec)				

IV. Data Analysis and Interpretation

A. Taking into account the data from sections III.A. and III.B., compare the amount of particle R before the reaction with that after the reaction. What conclusions can you draw from this information?

B. Write a balanced chemical equation for the overall reaction you observed. How does this reaction compare to the equation you wrote for section II.A.?

C. Using the data you collected in section III.C., propose the series of steps that describes the route taken (called the mechanism) by the reaction as it proceeds from reactants to products.

D. Describe what happens to particle R and RB as the reaction proceeds from reactants to products.

E. Determine the average rate of the reaction to produce eight product particles. Express this rate with respect to the appearance of product BG in units of [BG]/s.

F. Compare the rates of the reactions from sections II.B. and IV.E. How do you account for any differences you observe? What role do any of the reacting particles play in this difference?

G. A chemical substance that increases the rate of a chemical reaction but is neither a reactant nor product in the overall equation for the reaction is called a catalyst. Identify the catalyst in the reaction studied in this experiment. How does a catalyst increase the rate of a chemical reaction?

ACTIVATION ENERGY

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/KR2BN.htm

This will load a Graphics Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: How does the activation energy affect a chemical reaction?

I. Data Collection

Open the graphic simulation KR2BN:

http://introchem.chem.okstate.edu/DCICLA/KR2BN.htm

A. Use the information in the simulation to write an equation representing the hypothetical reaction being studied in this activity.

B. Sketch the reaction profile (reaction energy diagram) illustrated in the simulation. Label the sketch using the following terms: potential energy, reactants, products, reaction progress, activation energy, enthalpy, and collision energy. Determine values for the activation energy and enthalpy and include them in your diagram (since the activation energy is known, you can use proportions to estimate enthalpy).

C. Calibrate the time axis (x-axis) of the Strip Chart. To do this, click on the Resume button and with a stopwatch time how long it takes for the strip chart line to proceed across the graphing space. Measure the length of the line in millimeters (mm) with a ruler. Record your data in the spaces below. Do this two more times and calculate an average. Use the average to develop a formula for converting mm to seconds.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

Formula: 1 mm =	seconds
-----------------	---------

D. In the table below record the beginning concentrations of the reactants and products of the hypothetical reaction you are studying. Click on the Reset button. Click on the Enable Reactions button and the Resume button to begin the reaction. Allow the strip chart to proceed about one half of the way across the Strip Chart Region. Pause the reaction. Record the final concentrations and determine the elapsed time. Calculate the change in concentration and average rate during the elapsed time.

	[R ₂]	[B]	[R ₂ B]
Initial []			
Final []			
[]			
Time (sec)			
Average Rate			

E. Click on the Reset button. Assume that the hypothetical reaction you are studying has a different activation energy than the one you measured in section I.B. (Remember the reaction profile for a real chemical reaction cannot be adjusted without changing its mechanism. This simulation is only allowing a change in the activation energy to study the effect that activation energy has on the rate of chemical reactions.) Lower the activation energy by 2 kJ/mol and repeat the procedure of the previous section.

	[R ₂]	[B]	[R ₂ B]
Initial []			
Final []			
[]			
Time (sec)			
Average Rate			

F. Click on the Reset button. Lower the activation energy by another 2 kJ/mol and repeat the procedure of the previous section. (The easiest way to return the simulation to its default state if you have to start over is to use the refresh button of your browser to reload the software.)

	[R ₂]	[B]	[R ₂ B]
Initial []			
Final []			
[]			
Time (sec)			
Average Rate			
II. Data Analysis and Interpretation

A. What happens to the rate of a chemical reaction that has a lower activation energy? Use both the strip chart graph and your data points as evidence for your conclusion.

B. Explain why a lower activation energy has that effect.

III. Data Collection

Open the graphic simulation KR2GN:

http://introchem.chem.okstate.edu/DCICLA/KR2GN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar Region to construct the overall chemical equation for the reaction you are studying.

B. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

C. Turn your attention to the Reaction Viewer. Use the Reactions pull-down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

D. Sketch out the reaction profiles for each of the steps in the reaction mechanism. Label each of the profiles as you did in section I.B.

E. Click on the Reset button. Remove the Tolerence halo from the product molecule in the first step of the mechanism. (This is so that no reverse reaction can take place.) Adjust the amounts of the reactants and products so that you have only 5 moles of the reactant of the first step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Resume and then the Enable Reactions buttons to begin the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

F. Click on the Reset button. In the drop-down menu in the Module Control Region select Kinetics. Adjust the amounts of the reactants and products so that you have only 5 moles of the reactant of the first step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the step you are studying to estimate the rate of that step.

G. In the drop-down menu in the Module Control Region select Reaction Viewer. Click on the Reset button. Display the second step of the mechanism. Adjust the amounts of the reactants and products so that you have only 5 and 4 moles of the reactants of the second step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Resume and then on the Enable Reactions buttons to begin the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

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H. Click on the Reset button. In the drop-down menu in the Module Control Region select Kinetics. Adjust the amounts of the reactants and products so that you have only 5 and 4 moles of the reactants of the second step of the mechanism. Make sure that you have 0 moles of the other reactants and products. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the step you are studying to estimate the rate of that step.

IV. Data Analysis and Interpretation

Compare the rates of the two steps of the mechanism for the reaction. Why is one of the steps slower than the other? How are the rates of the steps related to the reaction profiles?

V. Data Collection

Use the Refresh button of your browser to restore the simulation to its original form. Click on the Reset button. In the drop-down menu in the Module Control Region select Kinetics. Click on the Enable reaction, Get Data, and Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Pick the change in concentration of the product of the overall reaction to calculate the rate of the reaction.

VI. Data Analysis and Interpretation

A. Compare the rate of the overall reaction with the rates of the individual steps in the mechanism. (See sections III.F. and H.)

B. What conclusion can you draw concerning the role that each step in a mechanism plays in the rate of a chemical reaction?

VII. Data Collection

Design experiments to investigate the relationship between the rate of production of the product R_2G and the initial concentrations of the reactants of the reaction you are studying. Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[]	[]	Initial Rate,[R ₂ G]/time

VIII. Data Analysis and Interpretation

- A. What effect does doubling the concentration of G have on the initial rate of the reaction?
- B. What effect does doubling the concentration of R have on the initial rate of the reaction?
- C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants R and G (see section IV.A.). Determine the rate constant for the reaction.

IX. Data Collection

Open the graphic simulation KB2RN:

http://introchem.chem.okstate.edu/DCICLA/KB2RN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar Region to construct the overall chemical equation for the reaction you are studying.

B. Turn your attention to the Reaction Viewer. Use the Reactions pull-down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

C. Design experiments to investigate the relationship between the rate of production of the product B_2R and the initial concentrations of the reactants of the reaction you are studying. Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[]	[]	Initial Rate, [B ₂ R]/time

X. Data Analysis and Interpretation

A. What effect does doubling the concentration of B have on the initial rate of the reaction?

B. What effect does doubling the concentration of R have on the initial rate of the reaction?

C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants B and R. Determine the rate constant for the reaction.

D. How would you characterize each step in the mechanism in terms of the number of the original reactant particles necessary for the stoichiometry of the reaction? How is this related to the rate law you proposed in section IX.? E. How would you characterize the number and kind of reactant particles necessary to determine the rate of the overall reaction? How does the mechanism explain why each reactant particle is necessary or not necessary to determine the rate?

F. Compare the rate laws for the reaction KR2GN with the reaction KB2RN. What are the differences in the mechanisms of the reactions that accounts for the differences in the rate laws?

KINETIC SYSTEMS

System 1

Investigate the mechanisms of chemical reactions:

A. $F_2 + NO_2 \rightarrow NO_2F + F$

Molecular-http://introchem.chem.okstate.edu/DCICLA/KNO2FM.htm

Graphic-http://introchem.chem.okstate.edu/DCICLA/KNO2FN.htm

B. $RB \rightarrow R+B$

Molecular—http://introchem.chem.okstate.edu/DCICLA/K2RBO2M.htm Graphic—http://introchem.chem.okstate.edu/DCICLA/ K2RBO2N.htm

C. $R+2G \rightarrow RG_2$

Molecular—http://introchem.chem.okstate.edu/DCICLA/KRG2M.htm Graphic—http://introchem.chem.okstate.edu/DCICLA/KRG2N.htm

D. For $RG \rightarrow R+G$

Molecular—http://introchem.chem.okstate.edu/DCICLA/KCATRGM.htm Graphic—http://introchem.chem.okstate.edu/DCICLA/KCATRGN.htm

System 2

Investigate the rate laws of chemical reactions. (See system 1 for examples.)

System 3

There are two possible mechanisms for $G_2 + 2B \rightarrow 2GB$:

 $G_2 + B \rightarrow GB + G$ slow

 $G+B \rightarrow GB$

 $G_2 \rightarrow G + G$ slow

 $G+B \rightarrow GB$

- A. Use the evidence from http://introchem.chem.okstate.edu/DCICLA/K2GBNa.htm to pick the correct mechanism.
- B. Use the evidence from http://introchem.chem.okstate.edu/DCICLA/K2GBNb.htm to pick the correct mechanism.

System 4

Investigate the effect that temperature has on the rate of a chemical reaction. (Hint: use the Arrhenius equation.)

System 5

Investigate the effect that activation energy has on the rate of a chemical reaction. (http://introchem.chem.okstate.edu/DCICLA/KR2BN.htm)

System 6

Investigate any other kinetic system or investigate a modification of any of the above systems.

RESEARCH STATEMENTS

Use evidence from the MoLE simulations to prove or disprove the following assertions.

Following are locations of various reactions that can be used in your investigations.

1. The amount of a catalyst does not affect the rate of a chemical reaction.

Molecular-http://introchem.chem.okstate.edu/DCICLA/KCATBGM.htm

Graphic-http://introchem.chem.okstate.edu/DCICLA/KCATBGN.htm

- 2. According to your textbook, increasing the temperature 10K will double the rate of a chemical reaction. This depends on the activation energy of the reaction. (http://introchem.chem.okstate. edu/DCICLA/KR2BN.htm)
- 3. According to your textbook, increasing the temperature 10K will double the rate of a chemical reaction. This depends on the H of the reaction. (http://introchem.chem.okstate.edu/DCICLA/ KR2BN.htm)

SHIFTING REACTIONS A

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ERGBM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: What are the characteristics of a hypothetical chemical reaction?

I. Data Collection

A. Open the Particulate Simulation. Use the pause button in the Control Bar region to stop the action of the particles. In the diagram below record the conditions of your sample as shown in the simulation.





B. Use the Reset button to refresh the screen. Determine the concentration (mol liter⁻¹) of each substance in the control bar region. (Show your work.) Click on the pause button to stop the motion of the particles. In the Control Bar region, change the number of moles of one of the substances present by adding one half a mole to the amount already there. Resume motion and describe what you observe in the strip chart and the Sample Window. C. Use the Reset button to refresh the screen. Click on the Enable Reactions button. After a short period of time has elapsed, click the Pause button. In the space below draw a picture of the strip chart. Label the lines of the strip chart with their identity (R, GB, RG, and B).

D. Resume the action. Observe how the concentrations of the particles in the sample change over time. How can you tell when the reaction is completed? What particles are present when the reaction is completed?

E. Use the Reset button to refresh the screen. Use the pull-down menu to change the graphical representation to the replay function. Click the Enable Reactions button to begin the reaction. Allow the reaction to proceed for a short period of time (10 sec–20 sec). Click the Pause button. Scroll the time index bar back to the point where only the reactant particles are present. Click on the forward arrow to roll the reaction forward in a step-wise manner to the point where the first new particle appears. Explain, in detail, the nature of that interaction. Include drawings and specify the orientation of all of the atoms in the interaction.

II. Data Analysis

Write a chemical equation representing the chemical interaction you observed. (Simplify the equation so that no common particles are on both sides of the equation and it represents the lowest ratio of whole numbers of particles.)

III. Data Collection

A. Use the Reset button to refresh the screen and the Pause button to stop the action. Using the controls in the Control Bar region, fix the amounts of R and GB at zero, of RG at 3, and B at 4. Set the graphics display to Concentrations, and resume the interaction. Calculate the concentrations of the particles. Calculate the initial concentrations of all the substances (R, GB, RG and B).

B. Click on the Enable Reactions button. When the reaction is complete, click on the Pause button. Calculate and record the final concentrations of all of the substances.

C. Use the Reset button to refresh the screen. Using the controls in the Control Bar region, fix the amounts of R and GB at zero, of RG at 3, and B at 4. Use the pull-down menu to change the graphical representation to the replay function. Click the Enable Reactions button to begin the reaction. Allow the reaction to proceed for a short period of time (10 sec–20 sec). Click the Pause button. Scroll the time index bar back to the point where only the reactant particles are present. Click on the forward arrow to roll the reaction forward in a step-wise manner to the point where the first new particle appears. Explain, in detail, the nature of that interaction. Include drawings and specify the orientation of all of the atoms in the interaction.

IV. Data Analysis

A. Write a chemical equation representing the chemical interaction you observed. (Simplify the equation so that no common particles are on both sides of the equation and it represents the lowest ratio of whole numbers of particles.)

B. Compare and contrast the two equations you wrote in sections II. and IV.A.

V. Interpretation and Conclusions

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A. Chemists refer to the type of reaction you have been investigating as a reversible reaction. Using the chemical system you investigated explain what is meant by reversible reaction.

B. An example of a non-reversible reaction is:

 $2\text{KClO}_3(s) \rightarrow 2\text{KCl}(s) + 3\text{O}_2(g)$

What is meant when the term non-reversible is used to describe this reaction?

C. When viewed at the macroscopic level in the laboratory, chemical reactions seem to stop changing after a period of time. How does this compare to your molecular observations in this activity? How do your observations at the molecular level explain what happens at the macroscopic level?

D. Mental Modeling: Using the Particulate Simulation program see if you can observe both chemical reactions studied in this activity to occur in the same window. Illustrate your observation by drawing a sequence of interactions that result in both reactions occurring sequentially.

E. Summarize in a few statements what are the characteristics of chemical reactions of the type studied in this activity.

SHIFTING REACTIONS B

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ERGBN.htm

This will load a Graphics Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

	9				P (atm):	67.94
	3 10	6	9	7410	V (L):	1.00
		Θ			n (mol R):	0.600
	0	0		74.0	n (mol BC):	0.700
		0			n (mol RG)	0.800
	5	0	6		n (mol 8).	0.900
		_	0		TOKE	275.25
	Res	uma)(Reset		Enable Rea	ctions)
	Reaction	Viewer				-
	leactions		R + BG -> 1	RG + B		4
	leactants		8	4	RG .	12
	Products		80	;	8	1
	•	D			Ø	
ĩ	lase Angle				Tolerence	
			Reactant A			
			Product A			
			Product 8			
0 0	uthored	by Kirk Hair	ies, John Gald	n, and j er, and	Michael Abr	aham.

Figure 1.

Problem Statement: How can concentration changes affect a chemical reaction?

I. Data Collection

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A. Open the Graphics Simulation program. Using the data from the Control Bar Region, enter the initial concentration of each substance in the equation, along with the initial pressure, volume and temperature into the table below.

EXPERIMENT #1:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I		_					
Concentration Change – C		_					
Ending Concentration – E		_					
Pressure							
Volume							
Temperature							

B. Click on the Resume and then the Enable Reactions button to begin the reaction. When the reaction appears to be complete, click Pause to stop the action. Record the values of the ending concentrations in the table in Section I.A. Calculate the change in concentration of each of the substances in the reaction. In the space below, draw the appearance of the strip chart and label the axes. If necessary, use the scrollbar located under the strip chart to move the chart back to the beginning of the reaction. Identify the chemical substance that corresponds to each of the colored lines.

II. Data Analysis and Interpretation

A. Mental Modeling: In the following boxes, draw pictures at the level of atoms and molecules that represents the initial and ending states of the reaction.



B. Explain what is happening to each of the reactant and product substances over time. How does the strip chart illustrate the changes you observe?

C. How can you tell when the reaction is complete? What substances are present when the reaction appears to be complete?

D. Considering the substances that are present when the reaction appears to be complete, why do the concentrations of the substances cease to change?

III. Data Collection

A. If necessary, click Pause to stop the action. If you moved the strip chart scrollbar in the previous section, shift it back to as far to the right as it will go. Use the ending concentrations of BG, RG and B from Experiment #1 (Section I.A.) as the initial concentrations in this experiment. Enter those values in the table below. In the Control Bar Region add R until its concentration is 2.0 M. Record this initial concentration of R in the table below. Click the Resume button. Observe how the concentrations of the substances change over time. When the reaction appears to be complete, click the Pause button. Record the values of the ending concentrations in this table and calculate the change in concentration of each of the substances in the reaction. Draw and label the appearance of the portion of the strip chart for this reaction. (NOTE: If necessary drag the Strip Chart scrollbar to the left.)

EXPERIMENT #2: Increase Reactant R to 2.0 M

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							

B. If you moved the Strip Chart scrollbar in the previous section, shift it back to as far to the right as it will go. Use the ending concentrations of R, RG and B from Experiment #2 as the initial concentrations in this experiment. Enter those values in the table below. In the Control Bar Region add BG until its concentration is 1.0 M. Record this initial concentration of BG in the table below. Click the Resume button. Observe how the concentrations of the substances change over time. When the reaction appears to be complete, click the Pause button. Record the values of the ending concentrations in this table and calculate the change in concentration of each of the substances in the reaction. Draw and label the appearance of the portion of the strip chart for this reaction. (NOTE: If necessary drag the Strip Chart scrollbar to the left.)

EXPERIMENT #3: Increase Reactant BG to 1.0 M

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C						-	
Ending Concentration – E							
-						-	

C. In a manner similar to the previous experiments, remove R until its concentration equals 0.75 M. Record the new initial conditions of all substances in the table below. Click the Resume button. Observe how the concentrations of the particles in the sample change over time. When the reaction is appears to be complete, click the Pause button. Record the values of the ending concentrations in the table and calculate the change in concentration of each of the substances in the reaction. Draw and label the appearance of the portion of the strip chart for this reaction.

EXPERIMENT #4: Decrease Reactant R to 0.75 M

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							

D. In a manner similar to the previous experiments add RG until its concentration is 2.0 M. Record the new initial conditions of all substances in the table below.

EXPERIMENT #5: Increase product RG to 2.0 M

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							

Before initiating the reaction draw what you think the Strip Chart Region will look like during this reaction in the box labeled Your Prediction.

Click the Resume button. Observe how the concentrations of the particles in the sample change over time. When the reaction appears to be complete click the Pause button. Record the values of the ending concentrations in the ICE table (above) and calculate the change in concentration of each of the substances in the reaction. Draw and label the appearance of the portion of the strip chart for this reaction in the Your Observation box. E. In a manner similar to the previous experiments remove RG until its concentration is 1.0 M. Record the new initial conditions of all substances in the table below.

EXPERIMENT #6: Decrease product RG to 1.0 M

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							

Before initiating the reaction, draw what you think the Strip Chart Region will look like during this reaction in the box labeled Your Prediction.

Your Prediction:	Your Observation:					

Click the Resume button. Observe how the concentrations of the particles in the sample change over time. When the reaction appears to be complete, click the Pause button. Record the values of the ending concentrations in the ICE table (above) and calculate the change in concentration of each of the substances in the reaction. Draw and label the appearance of the portion of the strip chart for this reaction in the Your Observation box.

IV. Data Analysis and Interpretation

A. Summarize your observations of Experiments #3–#6 by completing the table below. As an example, the entries for Experiment #2 have been done for you.

Experiment	Stress	Change in [Reactants]	Change in [Products]	Reaction shift
#2	Add reactant [R]	Concentrations decreased	Concentrations increased	Left to Right
#3				
#4				
#5				
#6				

2.0

B. Consider the strip chart recording on the right for a hypothetical experiment.

What was the stress placed on the reaction at time 2?



Write an equation to describe this reaction, then set up and complete all the entries in an ICE table.

V. Conclusions

A. Review the summary of your experimental observations that you prepared in Section IV.A. Write a statement(s) that generalizes how stressing a reaction by adding or removing a reactant or product shifts the chemical reaction.

B. Mental Modeling: Consider the strip chart recording on the right for a hypothetical experiment. Write an equation to describe this reaction, then set up and complete all the entries in an ICE table.



In the following boxes, draw pictures at the level of atoms and molecules that represents the progress of the hypothetical experiment from t=1 to t=2 to t=3. Indicate those particles that are added or subtracted from the sample as a result of the stress placed on the system.

time = 1	time = 2	time = 3

If you were to make a drawing for time=4, how would it be similar to the drawing you made for time=3? How would it be different?

EXTENT OF A CHEMICAL REACTION

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ERGBN.htm

This will load a Graphics Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

	000000000000000000000000000000000000000	0)++)++)++)++)++	P (atm): V (L) In (mol R): In (mol RC) In (mol RC) In (mol R): T (K):	67.94 1.00 0.600 0.700 0.800 0.900 275.25
		esuma	Reset		Enable Rea	ctions)
	Reaction	on Viewer	Participation			4
	Reaction	15	R + BG -> 1	0G + 8		(9)
	Reactan	ts.	8		8G	12
	Products	8	RC	1	5	- 2
	•	0		_	Ð	•
	Base An	gle	Reactant A Reactant B Product A		Tolerence	
0 0	Copyrig	M 2002 by	Product B Michael Abrahan	n, and j	john Geider	alt inte

Figure 1.

Problem Statement: What is the relationship between reactant and product concentrations at the end of a reaction?

I. Data Collection

Open the Graphic Simulation program for the R+BG reaction. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reaction buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #1:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	2.0		2.0		0		0
Concentration Change – C							
Ending Concentration – E							
Pressure							
Volume							
Temperature							

II. Data Analysis and Interpretation

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

B. Draw and label the appearance of the strip chart. Identify each kind of particle on the strip chart and explain what is happening to each over time. How does the strip chart illustrate the change in the data in the table?

III. Data Collection

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reactions buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #2:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	1.0		1.0		0		0
Concentration Change – C						_	
Ending Concentration – E							
Pressure							
Volume							
Temperature							

IV. Data Analysis and Interpretation

- A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.
- B. Draw and label the appearance of the strip chart. Identify each kind of particle on the strip chart and explain what is happening to each over time. How does the strip chart illustrate the change in the data in the table?

C. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R	+	BG	\rightarrow RG +	В
Initial Concentration – I	1.5		1.5	0	0
Concentration Change – C					
Ending Concentration – E					

V. Data Collection

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #3:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	1.5		1.5		0		0
Concentration Change – C							
Ending Concentration – E							
Pressure							
Volume							
Temperature							

VI. Data Analysis and Interpretation

- A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.
- B. Comment on how your predictions in IV.C. compared to the actual values determined from experiment.

C. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	0		0		1.0		1.0
Concentration Change – C							
Ending Concentration – E							

VII. Data Collection

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

EXPERIMENT #4:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I	0		0		1.0		1.0
Concentration Change – C							
Ending Concentration – E		_					
Pressure							
Volume							
Temperature							

VIII. Data Analysis and Interpretation

A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.

- B. Comment on how your predictions in VI.C. compared to the actual values determined from experiment.
- C. Compare your data in sections III. (Experiment #2) and VII. (Experiment #4). How do you explain this comparison?
- D. Given the initial concentrations in the following table, predict what the concentration change and ending concentrations would be. How did you make your predictions?

	R +	- BG -	→ RG +	В
Initial Concentration – I	2.0	0.5	0	0
Concentration Change – C				
Ending Concentration – E				

IX. Data Collection

Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume button to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations in the following table.

R	+	BG	\rightarrow	RG	+	В
2.0		0.5		0		0
	R 2.0	R + 2.0	R + BG 2.0 0.5	$\begin{array}{cccc} R & + & BG \rightarrow \\ 2.0 & 0.5 \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
X. Data Analysis and Interpretation

- A. Calculate the change in concentration of each of the particles in the reaction and record the values in the above table.
- B. Comment on how your predictions in VIII.D. compared to the actual values determined from experiment.

XI. Data Collection

A. Using the Control Bar region, adjust the initial conditions of the reaction being studied to those listed in the following table. Record the pressure, volume, and temperature of the sample in the following table. Use the Resume and Enable Reactions buttons to begin the reaction. When the reaction is completed, pause to stop the action. Record the values of the ending concentrations and the change in concentration of each of the particles in the following table.

R	+	BG	\rightarrow	RG	+	В
1.0		0.6		1.2		0.8
	R 1.0	R + 1.0	R + BG 1.0 0.6	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

B. Carry out two additional experiments by adjusting the concentrations of the reactants and products to values of your choosing. Be careful that the ending concentrations do not try to exceed the limits of the allowable values. Check to make sure the ending values of volume and temperature do not change.

EXPERIMENT #7:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							
Pressure							
Volume							
Temperature							

EXPERIMENT #8:	R	+	BG	\rightarrow	RG	+	В
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E							
Pressure							
Volume							
Temperature							

XII. Data Analysis

Summarize the ending concentrations of reactants and products for the eight reactions you studied in this activity by recording your data in the left-hand sections of the following table.

Pressure Volume Temperature			
		Calculation Resu	lts
	$R + BG \rightarrow RG + B \left[\right]$		
Experiment #1: Ending Concentration —E			
Experiment #2: Ending Concentration —E			
Experiment #3: Ending Concentration —E			
Experiment #4: Ending Concentration —E			
Experiment #5: Ending Concentration —E			
Experiment #6: Ending Concentration —E			
Experiment #7: Ending Concentration —E			
Experiment #8: Ending Concentration —E			

XIII. Data Interpretations and Conclusions

A. What conclusions can be drawn from these data? Find an algebraic equation that relates the ending concentrations of the reactants and products of the reaction studied. (Hint: Try all possible combinations of the four concentrations by multiplication and/or division. For example, multiply all four together, multiply two and divide by the other two, etc., looking for the combination that gives the most constant result.) Summarize your results for three possibilities in the table above. Label each column with how you combined the four concentrations in the box provided. Discuss your results below.

B. Use your results to predict the ending concentrations for the following. Show how you made your prediction. Check your prediction with the Graphic Simulation.

	$R + BG \rightarrow RG +$	- B
Initial Concentration – I	1.0 0.6 0	0
Concentration Change – C		
Ending Concentration – E		
Pressure		
Volume		
Temperature		

EQUILIBRIUM SYSTEMS

System 1

Investigate reactions other than the $R+BG \rightarrow B+RG$.

For $R+G \rightarrow RG$ go to:

Molecular-http://introchem.chem.okstate.edu/DCICLA/ERGM.htm

Graphic-http://introchem.chem.okstate.edu/DCICLA/ERGN.htm

For $BG \rightarrow B+G$ go to:

Molecular-http://introchem.chem.okstate.edu/DCICLA/EBGM.htm

Graphic-http://introchem.chem.okstate.edu/DCICLA/EBGN.htm

For $RB \rightarrow R+B$ go to:

Molecular-http://introchem.chem.okstate.edu/DCICLA/ERBM.htm

Graphic-http://introchem.chem.okstate.edu/DCICLA/ERBN.htm

System 2

Investigate the effect that temperature has on the shifting of exothermic (BG \rightarrow B+G) and endothermic (RB \rightarrow R+B) reactions (see system 1). Investigate how the value of K is affected.

System 3

Investigate the effect that pressure/volume has on the shifting of different reactions (see system 1). Investigate how the value of K is affected.

System 4

Investigate the relationships among K, T, and H. (Hint: use the van't Hoff equation.)

System 5

Investigate the relationships between K and Q for different kinds of concentration, pressure, and temperature changes.

System 6

Investigate the relationships between the rates of forward and reverse reactions as the reaction proceeds from initial to final states.

System 7

Investigate any other equilibrium system or investigate a modification of any of the above systems.

RESEARCH STATEMENTS

Use evidence from the MoLE simulations to prove or disprove the following assertions. Following are locations of various reactions that can be used in your investigations.

For $R + G \rightarrow RG$ go to:

Graphic-http://introchem.chem.okstate.edu/DCICLA/ERBN.htm

- 1. Temperature is the only factor that will affect the value of the equilibrium constant for a chemical reaction.
- 2. Reactions at equilibrium have concentrations related by stoichiometry.
- 3. At equilibrium, chemical reactions have equal concentrations of reactants and products.
- 4. The rates of chemical reactions slow as they go from initial states until they stop at the final state.
- 5. The changes in concentrations of reactants and products as the reaction proceeds from the initial state to the final state are controlled by the stoichiometry of the equation.

ACID/BASE CLASSIFICATIONS

Name

Section

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDSM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: What are the characteristics of acid solutions?

I. Data Collection

A. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Record your observations of what is happening. Use some or all of the following terms in your description: solution, solvent, solute, concentration, water, acid, base, reactant, and product. What is (are) the reactant(s) in this reaction? What is (are) the product(s) in this reaction?

B. Reset the simulation. Based on what you observe in the sample region and control bar region of the screen, calculate and record the concentration of each substance present in the following table before the reaction has taken place. Click on the Enable Reactions button. Allow the simulation to run until no more changes occur. Click on the Pause button and calculate and record the concentration of each substance present in the following table.

	[HG]	[H ₂ O]	[H ₃ O ⁺]	[G-]
Before Reaction				
After Reaction				

II. Data Analysis and Interpretation

A. Write a balanced chemical equation for the reaction you have observed in this simulation.

B. HG represents a class of chemical compound called an acid. Most common acids are found as water solutions. As a consequence, the reaction you wrote in section II.A. is called a hydrolysis reaction. These kinds of interaction can be characterized as transfers. What is being transferred in an acid solution? Where is it transferred? What is the result of the transfer?

C. Write a hydrolysis reaction for the acids HCl and for HNO₃.

- D. What chemical species do all of these acids have in common?
- E. Compare the concentration of the reactant acid with the concentration of the product compounds for the reaction in section II.B. What can you say about the extent of this reaction? Such compounds are called strong acids.

III. Data Collection

A. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDSN.htm

This will load the Graphic Simulation for the reaction you studied in the previous sections of this activity. If you haven't already done so, read the Numeric Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

B. Write the balanced equation for the reaction.

C. Before starting the simulation, fill in the Before Reaction row in the table below with the information requested.

	[HG]	[H ₂ O]	[H ₃ O ⁺]	[G-]
Before Reaction				
After Reaction				

- D. Click on the Resume and Enable Reactions buttons. Allow the simulation to run until no more changes occur. Click on the Pause button and record your observations. Fill in the After Reaction row in the previous table with the information requested.
- E. Reset the simulation and increase the amount of HG to 2.00 moles. Repeat the previous experiment and fill in the following table with the information requested.

	[HG]	[H ₂ O]	[H ₃ O ⁺]	[G-]
Before Reaction				
After Reaction				

IV. Data Analysis and Interpretation

A. Compare the concentration of the strong acid HG before the reaction has occurred with the concentration of H₃O⁺ after the reaction for both experiments. What was the extent of the reaction in each experiment? (What percentage of the HG was converted to H₃O⁺?)

B. For the reaction in section III.C., compare the concentration of water before the reaction with the concentration of HG before the reaction? What is the ratio of H₂O to HG?

C. For the reaction in section III.C., compare the concentration of water before the reaction with the concentration of water after the reaction? Discuss this comparison.

D. How much of the water actually reacts with the HG? What percentage of the total water is this?

E. What role does the water that doesn't react with the HG play in the reaction?

F. An alternate way of writing the equation for the reaction studied is to not include water. Why might you be justified in doing this? Write this equation.

V. Data Collection

Open the molecular simulation ACIDWM:

http://introchem.chem.okstate.edu/DCICLA/ACIDWM.htm

This is a Particulate Simulation for the acid HB.

A. Click on the Resume button and then the Enable Reactions button and allow the simulation to run. Use the replay function in the Module Display Region of the simulation to study the result of individual collisions between reactant and product particles. Record your observations of what is happening. Use some or all of the following terms in your description: solution, solvent, solute, concentration, water, acid, base, reactant, product, forward reaction, and reverse reaction. What is (are) the reactant(s) in this reaction? What is (are) the product(s) in this reaction?

B. Using the procedure you used to study the chemical reaction in the previous sections, fill in the table below with the information requested for this new chemical reaction.

	[HB]	[H ₂ O]	[H ₃ O ⁺]	[B-]
Before Reaction				
After Reaction				

C. Reset the simulation, and adjust the amounts of H_3O^+ and B^- to 3.0 moles each and the amount of HB to 0.0 moles. Using the procedure you used to study the chemical reaction in the previous sections, fill in the table below with the information requested.

	[H ₃ O ⁺]	[B ⁻]	[HB]	[H ₂ O]
Before Reaction				
After Reaction				

VI. Interpretation and Conclusions

A. Write a single balanced chemical equation (hydrolysis) that represents your observations in both sections V.B. and C.

B. What is the nature of this reaction? Compare the concentration of the reactant acid with the concentration of the product compounds for the reaction in section V. How would you characterize the extent of this reaction? How is it different from the reaction studied in section I. of this activity? Such compounds are called weak acids. C. What is being transferred in the reaction studied in section V.B.? What is being transferred in the reaction studied in section V.C.?

VII. Data Collection

Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDWN.htm

This will load the Graphic Simulation for the reaction you studied in the previous sections of this activity.

A. Using the data from the Control Bar Region, enter the initial concentrations of each substance in the equation into the table (called an ICE table) below.

	HB -	+	H_2O	\rightleftharpoons	$H_{3}O$	+	B-
Initial Concentration – I							
Concentration Change – C							
Ending Concentration – E		_					

- B. Click on the Resume and then the Enable Reactions buttons to begin the reaction. When the reaction appears to be complete, click Pause to stop the action. Record the values of the ending concentrations in the table in Section A. Calculate and record the change in numbers of moles of each of the substances in the reaction.
- C. Reset the simulation and adjust the beginning amount of HB to 0.750 moles. Repeat the experiment in the previous sections and complete the ICE table that follows.

	HB	+	$H_2O^+ \rightleftharpoons$	H ₃ O⁺	+	B^-
Initial Concentration – I						
Concentration Change – C						
Ending Concentration – E						

VIII. Interpretation and Conclusions

A. Compare the concentration of the weak acid HB before the reaction has occurred with the concentration of H₃O⁺ after the reaction for both experiments. What percentage of the HB was converted to H₃O⁺ in each experiment?

B. For the reaction in section VII.A., compare the concentration of water before the reaction with the concentration of HB before the reaction? What is the ratio of H₃O⁺ to HB?

C. For the reaction in section VII.A., compare the concentration of water before the reaction with the concentration of water after the reaction? Discuss this comparison. What role does the water that doesn't react with the HB play in the reaction?

D. Considering the change in concentration, would you be justified in ignoring the concentration of water in determining the dissociation constant (equilibrium constant, K_a) of HB? Why or why not? Write an alternate equation for the reaction that doesn't include water.

E. Determine the dissociation constants (K_a) for HB for both experiments in section VII. Compare the values you obtain.

ACID/BASE INTERACTIONS

Name

SECTION

Log on to the Internet. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDS+BM.htm

This will load a Particulate Simulation. Once you have the simulation running, your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Figure 1.

Problem Statement: How do acids and bases interact?

I. Data Collection

A. The simulation represents the strong acid HG when it is added to water. Allow the acid and water to interact by clicking on the Resume and Enable Reactions buttons. Describe what happens when the acid dissolves in the water. Use the Replay function in the drop-down menu and the tracking button to aid your observations. Write a balanced equation to represent the interaction. What chemical species are present when the interaction is complete?

B. Pause the simulation. Add 1.00 mole of OH⁻ to the reaction container. Based on what you observe in the Sample Region and Control Bar Region of the screen, calculate and record the initial concentration of each substance present in the following table. Click on the Resume button. Allow the simulation to run until no more changes occur. Click on the Pause button and calculate and record the ending concentration of each substance present in the following table. Calculate and record the change in concentration for each of the substances.

	[H ₂ O]	[HG]	[H ₃ O ⁺]	[G⁻]	[OH⁻]
Initial – I					
Change – C					
Ending – E					

C. Add an additional 1.0 mole of OH⁻ to the reaction container. Click on the Resume button and observe the interactions between the reactant particles. Use the Replay function in the drop-down menu to aid your observations. Describe what happened when the reactant particles interacted with each other. What interactions cause changes to occur and what interactions don't cause changes to occur?

II. Data Analysis and Interpretation

A. Write a balanced chemical equation for the reaction you observed in section I.B. and C. of this simulation.

B. How did you decide when the reaction was complete in section I.A.?

C. How did you decide when the reaction was complete in section I.B. and C.?

III. Data Collection

A. Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDS+BN.htm

This will load the Graphic Simulation for the reaction you studied in the previous sections of this activity. If you haven't already done so, read the Numeric Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

B. The simulation represents the strong acid HG when it is added to water. Allow the acid and water to interact by clicking on the Resume and Enable Reactions buttons. Describe what happens when the acid dissolves in the water. Write a balanced equation to represent the interaction. What chemical species are present when the interaction is complete?

C. Pause the simulation. Add 1.50 mole of OH⁻ to the reaction container. Based on what you observe in the Control Bar Region of the screen, calculate and record the initial concentration of each substance present in the following table. Click on the Resume button. Allow the simulation to run until no more changes occur. Click on the Pause button and calculate and record the ending concentration of each substance present in the following table. Calculate and record the change in concentration for each substance.

	[H ₂ O]	[HG]	[H ₃ O ⁺]	[G⁻]	[OH⁻]
I					
С					
E					

IV. Data Analysis and Interpretation

A. Using the data from section III.C. write a chemical equation representing the reaction you are studying.

B. What is the reacting capacity of this acid? (i.e., How much base is necessary to react with a specified amount of acid?)

C. What role does the water in the reaction container play? (What does the water do in the reaction?)

D. Discuss the change in concentration for each of the substances in the reaction. (Why does the change happen the way it does?)

V. Data Collection

Open the molecular simulation ACIDW+BM:

http://introchem.chem.okstate.edu/DCICLA/ACIDW+BM.htm

This will load a Particulate Simulation.

A. The simulation represents the weak acid HB when it is added to water. Allow the acid and water to interact by clicking on the Resume and Enable Reactions buttons. Describe what happens when the acid dissolves in the water. Use the Replay function in the drop down menu, the strip chart, and the tracking button to aid your observations. Write a balanced equation to represent the interaction. What chemical species are present when the interaction is complete?

B. Pause the simulation. Add 1.00 mole of OH⁻ to the reaction container. Based on what you observe in the sample region and control bar region of the screen, calculate and record the initial concentration of each substance present in the following table. Click on the Resume button. Allow the simulation to run until the reaction is complete. Click on the Pause button and calculate and record the ending concentration of each substance present in the following table. Calculate and record the change in concentration for each substance.

	[H ₂ O]	[HB]	[H ₃ O ⁺]	[B ⁻]	[OH⁻]
I	—				
С					
E					

C. Add an additional 1.00 mole of OH⁻ to the reaction container. Click on the Resume button and observe the interactions between the reactant particles. Use the Replay function in the drop down menu, the values in the Slide Bar region, the tracking function, and the strip chart to aid your observations. Describe what happens when the reactant particles interact with each other. What interactions cause changes to occur and what interactions don't cause changes to occur?

VI. Interpretation and Conclusions

A. Why was water not included in the table in section V.B.?

B. Write balanced chemical equations that represent all of your observations in both sections V.B. and C.

VII. Data Collection

Type the following address into the location-input line of your browser:

http://introchem.chem.okstate.edu/DCICLA/ACIDW+BN.htm

This will load the Graphic Simulation for the reaction you studied in the previous sections of this activity.

A. Using the data from the Control Bar Region, enter the initial concentrations of each substance in the equation into the table (called an ICE table) below.

	HB	+	H_2O	\rightleftharpoons	$\mathrm{H_{3}O^{*}}$	+	B-
Initial Concentration – I				_		_	
Concentration Change – C				_		_	
Ending Concentration – E							

B. Click on the Resume and then the Enable Reactions buttons to begin the reaction. When the reaction appears to be complete, click Pause to stop the action. Record the values of the ending concentrations in the table in Section A. Calculate and record the change in concentration of each of the substances in the reaction.

C. Pause the simulation. Add 0.128 mole of OH⁻ to the reaction container. Based on what you observe in the Control Bar Region of the screen, calculate and record the concentration of each substance present initially in the following table. Click on the Resume button. Allow the simulation to run until no more changes occur. Click on the Pause button and calculate and record the ending concentration of each substance present in the following table. Calculate the change in concentration for each substance.

	[H ₂ O]	[HB]	[H ₃ O ⁺]	[B-]	[OH ⁻]
I					
С					
E					

D. Reset the simulation. Click on the Resume and then the Enable Reactions buttons to generate the initial conditions for the acid base interaction. Pause the simulation. Add 1.50 mole of OH⁻ to the reaction container. Based on what you observe in the Control Bar Region of the screen, calculate and record the concentration of each substance present initially in the following table. Click on the Resume button. Allow the simulation to run until no more changes occur. Click on the Pause button and calculate and record the ending concentration of each substance present in the following table. Calculate the change in concentration for each substance.

	[H ₂ O]	[HB]	[H ₃ O ⁺]	[B ⁻]	[OH⁻]
I					
С					
E					

VIII. Interpretation and Conclusions

A. Compare the concentration of the weak acid HB before the reaction has occurred in section VII.A. with the concentration of H_3O^+ after the reaction in section VII.D. What percentage of the HB was converted to H_3O^+ ?

B. What is the reacting capacity of this acid? (i.e., How much base is necessary to react with a specified amount of the weak acid.) Compare the reacting capacity of the weak acid HB (section VII.) with the strong acid HG you studied in section III (also see section IV.B.).

C. Write balanced chemical equations that represent all of your observations in section VII.

D. Discuss the change in concentration for each of the substances in the reaction in VII.D. (Why does the change happen the way it does?)

- E. How would you explain to another student the difference between a strong acid and a weak acid with respect to:
 - a. the pH of a 0.100 M solution;
 - b. the [H⁺] compared to the initial concentration of the acid;
 - c. the magnitude of K_a;
 - d. the reacting capacity of the acid.

ACID/BASE SYSTEMS

Name

LAB SECTION

System 1

Investigate the properties of weak bases.

http://introchem.chem.okstate.edu/DCICLA/BASEW+AM.htm

http://introchem.chem.okstate.edu/DCICLA/BASEW+AN.htm

System 2

Investigate the acid properties of strong and weak polyprotic acids.

http://introchem.chem.okstate.edu/DCICLA/AcidPolyS.htm

http://introchem.chem.okstate.edu/DCICLA/AcidPolyW.htm

System 3

Investigate any other acid/base system or investigate a modification of any of the above systems.

RESEARCH STATEMENTS

Use evidence from the MoLE simulations to prove or disprove the following assertions. Following are locations of various reactions that can be used in your investigations.

- 1. A more dilute weak acid will have greater conductivity (i.e., will have a greater concentration of ions).
- 2. The greater the concentration of a weak acid, the greater the percentage of dissociation of the acid into ions.
- 3. The acid dissociation constant for a weak acid is dependent on concentration.
- 4. The acid dissociation constant for a weak acid is dependent on temperature.
- 5. Acid strength and acid concentration are the same concept for both strong and weak acids.
- 6. A strong diprotic acid has a $[H_3O^+]$ twice the value of a monoprotic acid.

Introduction to Laboratory Simulations



In the following activities you will examine chemical concepts in a simulated laboratory setting. To do these activities, you will need to make sure your browser has the latest plug-in to Macromedia Flash and Shockwave. Go to the Macromedia website at http://www.adobe.com/downloads/ to obtain them.*

^{*} The software used in these laboratory simulations was developed and programmed by Thomas Greenbowe, Han-ChinLiu and Rohini Vanchiswaran. © Thomas Greenbowe, September 2001 – Project supported by NSF-CCLI-EMD #0088709.

IODINE CLOCK

Name

Section

Problem Statement: How do concentration and temperature influence the rate of a chemical reaction?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/iodine_clock.html and open the Iodine Clock Simulation. Your screen should look like the figure.



The reaction to be investigated occurs in the beaker when four colorless solutions from four graduated cylinders are mixed. Different amounts of the solutions can be added together at a specified temperature. Radio buttons control these amounts and the temperature. A timer can be used to monitor how long it takes for a chemical reaction to use up one of the reactants.

The series of chemical interactions that take place follows:

$$3 I^{-}(aq) + S_{2}O_{8}^{2-}(aq) \to 2 SO_{4}^{2-}(aq) + I_{3}^{-}(aq)$$
(1)

$$I_{3}^{-}(aq) + S_{2}O_{3}^{2-}(aq) \to 3 I^{-}(aq) + S_{4}O_{6}^{2-}(aq)$$
(2)

 $2 I_{3}^{-} (aq) + \text{Starch} \rightarrow \text{Blue/Black Complex} + I^{-} (aq)$ (3)

The first reaction produces I_3^- . When I_3^- comes in contact with starch (in reaction three) it produces a characteristic blue/black color. However, before that can happen, $S_2O_3^{2-}$ reacts with it to produce color-less products (in reaction two). Because reaction two is much faster than reaction three, the third reaction won't take place until all of the $S_2O_3^{2-}$ is used up. Once that occurs, the colorless solution changes color.

B. If necessary, use the buttons to adjust the volume of KI (aq) to 12 mL and $(NH_4)_2S_2O_8$ (aq) to 30 mL. Then adjust the volume of water so that the sum of all the solutions when combined equals 100 mL. Make sure the temperature is set at 25 °C. Click on the start button. When the last solution is added, click to start the timer. Pause the timer when the reaction solution changes color. Record your data in the following table.

TRIAL	1.0 M KI (aq)	0.1 M (NH ₄) ₂ S ₂ O ₈ (aq)	Time @ 25 °C	Time @ 45 °C	Time @ 5 °C
1	12 mL	30 mL			
2	6 mL	30 mL			
3	12 mL	15 mL			

C. Adjust the amounts and temperatures of the reactants specified in the preceding table and repeat the general procedure of the preceding section. Record your data in the table.

II. Data Analysis and Interpretation

A. From the data you collected in the table from section I.B., calculate the molar concentration of I⁻, [I⁻], and $S_2O_8^{2-}$, $[S_2O_8^{2-}]$ for each trial and record your results in the following table.

TRIAL	[1-]	[S ₂ O ₈ ²⁻]	Ave Rate @ 25 °C	Ave Rate @ 45 °C	Ave Rate @ 5 °C
1					
2					
3					

- B. The rate of a chemical reaction is inversely proportional to the amount of time it takes for the reaction to happen. (If it takes half the amount of time, its rate is twice as big.) Calculate the average rate of each trial (time⁻¹) and record your results in the preceding table.
- C. Relate the change in [I⁻] to the change in average rate. How are they related? Are the changes directly proportional? What trials did you use to come to your conclusions?

D. Relate the change in $[S_2O_8^{2-}]$ to the change in average rate. How are they related? Are the changes directly proportional? What trials did you use to come to your conclusions?

E. On the following graph, or using a graphing program, plot the relationship between the temperature of the reactants and the rate of the reaction in trial 1. What happens to the rate of a chemical reaction as the temperature changes? What is the nature of this relationship? Are the changes directly proportional? (Optional: How are they related mathematically? Using a graphing program plot the amount of rate vs. the temperature. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line.)



III. Conclusions

A. Make a generalization of how concentration changes affect the rate of a chemical reaction.

B. Make a generalization of how temperature changes affect the rate of a chemical reaction.
CONCENTRATION/TEMPERATURE EFFECTS

Name

Section

Problem Statement: How do concentration and temperature influence the rate of a chemical reaction?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/kinetics.html and open the Concentration/Temperature Effects Simulation. Your screen should look like the figure.



The reaction to be investigated occurs in the beaker when four colorless solutions from four graduated cylinders are mixed. Different amounts of the solutions can be added together at different specified temperatures. Radio buttons control these amounts and the temperature. A timer can be used to monitor how long it takes for the chemical reaction to proceed to the same level of completeness as the standard solution contained in a second reference beaker.

The chemical interactions that takes place is:

$$3I^{-}(aq) + H_{2}O_{1}(aq) + 2H^{+}(aq) \rightarrow I_{3}^{-}(aq) + 2H_{2}O(l)$$

The reactant solutions are colorless. The product, I_3^- , is colored. As the reaction proceeds, the intensity of the color increases, indicating that the concentration of the products is increasing. The reaction is slow enough so that the time it takes to get to predetermined color intensity, and therefore a specific I_3^- concentration can be conveniently timed. A standardized solution is available so that the colors can be matched.

B. If necessary, use the buttons to adjust the volume of the reactant solution to the amounts shown in the following table. Notice that the volume of water is adjusted so that the sum of all the solutions when combined equals 100 mL. Make sure the temperature is set at 25 °C. Click on the start button. When the last solution is added, click to start the timer. Pause the timer when the reaction solution changes to a color that matches the color of the standard solution. Record your data.

TRIAL	H ₂ O (I)	0.010 M H ₂ O ₂ (aq)	1.0 M HCl (aq)	0.050 M KI (aq)	Time @ 25 °C
1	60 mL	10 mL	20 mL	10 mL	
2					
3					
4					
5					
6					
7					
8					

C. Design trials to test the effect that changing the concentration of each of the reactants has on the rate of the reaction by varying the amounts of the reactants. Try and minimize the number of trials tried. Record the conditions of each trial in the table above. Remember to adjust the amount of water so that each trial has 100 mL of total solution. Enter the parameters of each trial in the simulation and determine the amount of time it takes for each trial to reach the standard color. Record your data in the above table.

II. Data Analysis and Interpretation

A. From the data you collected in the table from section I.B. calculate the molar concentrations of H_2O_2 , $[H_2O_2]$, H^+ , $[H^+]$, and I^- , $[I^-]$, for each trial and record your results in the following table.

TRIAL	[H ₂ O ₂]	[H+]	[1-]	Rate @ 25 °C
1				
2				
3				
4				
5				
6				
7				
8				

- B. The rate of a chemical reaction is inversely proportional to the amount of time it takes for the reaction to happen. (If it takes half the amount of time its rate is twice as big.) Calculate the average rate of each trial (time⁻¹) and record your results in the preceding table.
- C. Relate the change in $[H_2O_2]$ to the change in average rate. How are they related? Are the changes directly proportional? What trials did you use to come to your conclusions?

- D. Relate the change in [H⁺] to the change in average rate. How are they related? Are the changes directly proportional? What trials did you use to come to your conclusions?
- E. Relate the change in [I⁻] to the change in average rate. How are they related? Are the changes directly proportional? What trials did you use to come to your conclusions?

III. Data Collection

Using the concentrations of trial 1 from section I.B., copy the rate for 25 °C into the following table. Repeat the experiment using the trial 1 concentrations at each of the specified temperatures. Calculate and record the rates in the following table.

TRIAL	[H ₂ O ₂]	[H+]	[1-]	Rate @ 5 °C	Rate @ 15 °C	Rate @ 25 °C	Rate @ 35 °C	Rate @ 45 °C
1								

IV. Data Analysis and Interpretation

On the following graph, or using a graphing program, plot the relationship between the temperature of the reactants and the rate of the reaction in trial 1. What happens to the rate of a chemical reaction as the temperature changes? What is the nature of this relationship? Are the changes directly proportional? (Optional: How are they related mathematically? Using a graphing program, plot the amount of rate vs. the temperature. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line.)



V. Conclusions

A. Make a generalization of how concentration changes affect the rate of a chemical reaction.

B. Make a generalization of how temperature changes affect the rate of a chemical reaction.

DECOMPOSITION OF H₂O₂

Name

Section

Problem Statement: How do catalysts influence the rate of a chemical reaction?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/rxnRate01.html and open the Decomposition of H₂O₂ Simulation. Your screen should look like the figure.



The apparatus is used to study the decomposition of hydrogen peroxide:

 $2 \ \mathrm{H_2O_2} \ (aq) \rightarrow 2 \ \mathrm{H_2O} \ (l) + \mathrm{O_2} \ (g)$

A flask is attached to a gas-measuring device that monitors the generation of oxygen gas. The rate at which oxygen gas is produced by the chemical reaction is a measure of the rate of the chemical reaction. Click on the gray rectangle to set up the reaction conditions. You will be asked to specify the amount of 3% H₂O₂, what potential catalyst you will try, and the amount of catalyst. Radio buttons control the amounts. Water is automatically added to make all of the solutions have equal total volumes. When you click on the start button, a magnified view of the graduated gas-measuring devise allows you to see how much gas is being collected over time. You can also click onto graphs that plot the generation of O₂ gas or the consumption of H₂O₂ solution. Try this out to see how this works.

B. Reset the apparatus. Measure the rate of the dissociation of 5.0 mL of uncatalyzed H_2O_2 .

To do this, click on the set up rectangle, choose 5 mL of H₂O₂, choose 0.5 M KI, and choose 0 mL.

You have several options for timing the reaction: (1) Use a stopwatch to time how long it takes for a specified amount of O_2 gas to be produced. Express this as an average rate (in mL per second). Click on the start button and start the stopwatch at zero gas and stop the stopwatch at the specified volume. (2) Use the O_2 plot to see how long it takes to generate a specified amount of O_2 gas. Click on the Plot O_2 button to view the graph. Use the graph to determine the average rate by determining the slope of a straight line drawn between zero and the specified volume of gas. Record your data in the following table.

	Rate with 0.5M KI (mL/sec)		Rate with 1.0 M KCl (mL/sec)		Rate with 0.1 M FeCl ₃ (mL/sec)	
	0mL	2mL	0 mL	2mL	0 mL	2mL
5 mL H ₂ O ₂						
10mL H ₂ O ₂						

C. Repeat the experiment for all of the conditions specified in the above table and record your results. Sketch the plot for the generation of O, when 2 mL of KI is added to 5 mL of H₂O₂.

II. Data Analysis and Interpretation

A. Use the plot from section I.C. to describe what happens to the rate of this reaction as the reaction proceeds.

B. Relate the change in [H₂O₂] to the change in average rate. How are they related? Are the changes directly proportional?

C. Which of the substances that you added to H_2O_2 acted as a catalyst? Which was the best catalyst? What ion (ions) was (were) responsible for the catalytic effect? How did you eliminate other ions?

ACID/BASE pH

Name

Section

Problem Statement: What are the acid and base properties of solutions?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/ph_meter.html and open the Acid/Base pH Simulation. Your screen should look like the figure.



This simulation contains a pH meter. You can test the pH of strong and weak acid, base and salt solutions of different concentrations. You will set up the conditions of each measurement using the radio buttons and then insert the pH probes into the solution to obtain the pH of the solution. B. Under the acid solutions, choose HCl. Set the concentration of the solution at 1.00×10^{-2} M (use the slider bar or key in 1.00 and then the radio button). Set the volume at 100 mL (use the slider bar). Click on the Insert Probes button on the pH meter. Enter your pH data in the following table.

Solution	Concentration (M)	рН	[H+]	% Dissociated
HCl (aq)	1.00 × 10 ⁻²			
HCI (aq)	$1.00 imes 10^{-3}$			
HCI (aq)	$1.00 imes 10^{-5}$			

C. Remove the probes. Adjust the conditions of your measurements and measure the pH of each of the concentrations for the HCl solutions in the above table and enter the pH data you obtain.

II. Data Analysis and Interpretation

- A. pH is defined by the equation: $pH = -log [H^+]$. Calculate the $[H^+]$ for each of the conditions in the table in the previous section and record your results in the table.
- B. Compare the [H⁺] with the original concentration of HCl. What does this tell you about the amount of HCl present in the solution? What is the percentage of HCl that has dissociated (ionized) when it is dissolved in water? (Acids that have this characteristic are called strong acids.) Enter these values in the above table.

C. Write an equation representing the reaction when HCl is dissolved in water.

III. Data Collection

A. Under the acid solutions, choose $HC_2H_3O_2$. Set the concentration of the solution at 1.00×10^{-2} M (use the slider bar or key in 1.00 and then the radio button). Set the volume at 100 mL (use the slider bar). Click on the Insert Probes button on the pH meter. Enter your pH data in the following table.

Solution	Concentration (M)	рН	[H+]	% Dissociated
HC ₂ H ₃ O ₂ (aq)	$1.00 imes 10^{-2}$			
HC ₂ H ₃ O ₂ (aq)	$1.00 imes 10^{-3}$			
$HC_2H_3O_2$ (aq)	1.00 × 10 ⁻⁵			

B. Remove the probes. Adjust the conditions of your measurements and measure the pH of each of the concentrations for the HC₂H₃O₂ solutions in the above table and enter the pH data you obtain.

IV. Data Analysis and Interpretation

A. Calculate the [H⁺] for each of the conditions in the table in the previous section and record your results in the table.

- B. Compare the [H⁺] with the original concentration of HC₂H₃O₂. What does this tell you about the amount of HC₂H₃O₂ present in the solution? What is the percentage of HC₂H₃O₂ that has dissociated (ionized) when it is dissolved in water? (Acids that have this characteristic are called weak acids.) Enter these values in the above table.
- C. Compare the percent dissociation for the 1×10^{-2} M concentrations of HCl and HC₂H₃O₂. Generalize the relationship between the concentration of an acid and the % dissociation: for a strong acid, and for a weak acid.

D. Write an equation representing the reaction when HC₂H₃O₂ is dissolved in water.

V. Data Collection

A. Under the acid solutions, choose H_2SO_4 . Set the concentration of the solution at 1.00×10^{-2} M (use the slider bar or key in 1.00 and then the radio button). Set the volume at 100 mL (use the slider bar). Click on the Insert Probes button on the pH meter. Enter your pH data in the following table.

Solution	Concentration (M)	рН	[H+]
H ₂ SO ₄ (aq)	$1.00 imes 10^{-2}$		
H ₂ SO ₄ (aq)	$1.00 imes 10^{-3}$		
H ₂ SO ₄ (aq)	$1.00 imes 10^{-5}$		

B. Remove the probes. Adjust the conditions of your measurements and measure the pH of each of the concentrations for the H_2SO_4 solutions in the above table and enter the pH data you obtain.

VI. Data Analysis and Interpretation

- A. Calculate the [H⁺] for each of the conditions in the table in the previous section and record your results in the table.
- B. Compare the $[H^+]$ with the original concentration of H_2SO_4 . What does this tell you about the amount of H_2SO_4 present in the solution? What is the percentage of H_2SO_4 that has reacted when it is dissolved in water? Is H_2SO_4 a strong or weak acid?

C. Write an equation representing the reaction when H_2SO_4 is dissolved in water.

VII. Data Collection and Analysis

A. Using the procedure of the previous sections, measure the pH of 1.00×10^{-2} M concentrations of each of the acids in the list. Record your findings in the following table.

Solution	Concentration (M)	рН	[H+]	Strong/Weak
HCl (aq)	$1.00 imes 10^{-2}$			
H ₂ SO ₄ (aq)	1.00 × 10 ⁻²			
$HC_2H_3O_2$ (aq)	1.00 × 10 ⁻²			
HF (aq)	1.00 × 10 ⁻²			
$HC_{3}H_{5}O_{3}$ (aq)	1.00 × 10 ⁻²			
HNO ₃ (aq)	1.00 × 10 ⁻²			
HClO ₂ (aq)	1.00 × 10 ⁻²			
HNO ₂ (aq)	1.00 × 10 ⁻²			

B. Calculate the [H⁺] of each solution and classify each acid as weak or strong. Enter your findings in the previous table.

VIII. Data Collection

A. Under the base solutions, choose NaOH. Set the concentration of the solution at 1.00×10^{-2} M (use the slider bar or key in 1.00 and then the radio button). Set the volume at 100 mL (use the slider bar). Click on the Insert Probes button on the pH meter. Enter your pH data in the following table.

Solution	Concentration (M)	рН	[H+]	[OH-]
NaOH (aq)	1.00×10^{-2}			
NaOH (aq)	$1.00 imes 10^{-3}$			
NaOH (aq)	$1.00 imes 10^{-5}$			

B. Remove the probes. Adjust the conditions of your measurements and measure the pH of each of the concentrations for the NaOH solutions in the above table and enter the pH data you obtain.

IX. Data Analysis and Interpretation

A. Calculate the [H⁺] for each of the conditions in the table in the previous section and record your results in the table.

B. In a water solution the [H⁺] is related to the [OH⁻] by the following equation:

$$1 \times 10^{-14}$$
 = [H⁺] [OH⁻]

Use this equation to calculate the [OH-] of the NaOH solutions. Enter your results in the previous table.

- C. Compare the [OH-] with the original concentration of NaOH. What does this tell you about the amount of NaOH present in the solution? What is the percentage of NaOH that has reacted when it is dissolved in water? Is NaOH a strong or weak base?
- D. Write a chemical equation to represent what happens when NaOH dissolves in water.

X. Data Collection and Analysis

A. Using the procedure of the previous sections, measure the pH of 1.00×10^{-2} M concentrations of each of the bases in the list. Record your findings in the following table.

Solution	Concentration (M)	рН	[H+]	[Он-]	Strong/Weak
NaOH (aq)	1.00 × 10 ⁻²				
KOH (aq)	1.00×10^{-2}				
NH ₃ (aq)	1.00 × 10 ⁻²				
Ca(OH) ₂ (aq)	1.00×10^{-2}				
(CH ₃) ₂ NH (aq)	1.00 × 10 ⁻²				
$C_6H_5NH_2$ (aq)	1.00 × 10 ⁻²				
HONH ₂ (aq)	1.00 × 10 ⁻²				

B. Calculate the [H⁺] and [OH⁻] of each solution and classify each base as weak or strong. Enter your findings in the previous table.

ACID/BASE TITRATIONS

Name

Section

Problem Statement: How do acids and bases interact?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/acid_base.html and open the Acid/Base Titration Simulation. Your screen should look like the figure.



This simulation contains a titration apparatus. You can set up the conditions for a titration by following the step-by-step decisions in order by the numbers that are displayed in the simulation. As a trial: (1) select the strong acid vs. strong base reaction, (2) fill the burette with acid, (3) select HCl as your acid and KOH as your base, and (4) select bromothymol blue as your indicator. Click on the slider bar that adds acid to the flask. (A new button labeled Concordant Values appears.) Then add acid in 5 mL increments until the color changes in the flask. You can add acid dropwise by using the Dropwise button. You can repeat the titration using the same conditions by clicking on the Concordant Values button.

B. Reset the simulation. (1) Select the strong acid vs. strong base reaction, (2) fill the burette with acid, (3) select HCl as your acid and KOH as your base, and (4) select bromothymol blue as your indicator. Click on the slider bar that adds acid to the flask. Add acid in 5 mL increments until the color changes in the flask. Click on the Concordant Values button and re-enter the amount that was 5 mL less than the amount added that changed the color of the solution. Add the acid dropwise until one drop of acid just changes the color. Record the amount of added acid, the molarity of the base, and volume of the base in the table below. Calculate the molarity of the acid and enter the value in the provided space in the simulation. Check the accuracy of your calculation and then enter this value in the following table. Do not reset the simulation!

	Acid, HCl	Base, KOH
Volume (mL)		
Concentration (M)		

C. Click on the Graph button and sketch the graph in the space below.

D. Return to the titration apparatus. Click on the Concordant Values button and change the indicator to methyl red. Determine the amount of acid necessary to change the color of the solution. Enter the values in the table below. Do not reset the simulation!

	Acid, HCl	Base, KOH
Volume (mL)		
Concentration (M)		

E. Click on the Concordant Values button and change the base to Ba(OH)₂. Determine the amount of acid necessary to change the color of the solution. Enter the values in the table below.

	Acid, HCl	Base, Ba(OH) ₂
Volume (mL)		
Concentration (M)		

II. Data Analysis and Interpretation

A. Finish writing the chemical equation representing the reaction between HCl and KOH from section I.B.

 $\mathrm{HCl}(aq) + \mathrm{KOH}(aq) \rightarrow$

B. Rewrite the above equation as a net ionic equation.

C. Compare the amount of base necessary to react with HCl in sections I.B. and D.

Acid/Base Indicator	pH Range	Color change	
Methyl Red	4.8-6.0	Yellow to Red	
Bromothymol Blue	6.0–7.6	Yellow to Blue	

D. Indicators change colors at different pH ranges. The two indicators available for this part of the experiment are in the following table with their pH ranges.

Considering the differences in the pH ranges of methyl red and bromothymol blue, how do you account for the results of section I.B. and D. (Hint: use the plot in section I.C. in your explanation.)

E. Compare the amount of base necessary to react with HCl in sections I.B. and E. How do you account for any differences you observe? Write chemical equations to illustrate your conclusions.

F. Predict what volume of acid would have been necessary to change the color of the base solution in section I.B. if H₂SO₄ had been used instead of HCl. Explain your answer.

G. Sketch the graph that you would have generated if you had filled the burette with base and had the acid in the flask in section I.B.

III. Data Collection

A. Reset the simulation. (1) Select the weak acid vs. strong base reaction, (2) fill the burette with base, (3) select CH_3COOH as your acid and KOH as your base, and (4) select phenolphthalein as your indicator. Determine the amount of base necessary to change the color of the solution. Enter the values in the table below. Do not reset the simulation!

	Acid, CH ₃ COOH	Base, KOH
Volume (mL)		
Concentration (M)		

B. Click on the Graph button and sketch the graph in the space below.

IV. Data Analysis and Interpretation

A. Write the chemical equation representing the reaction between CH₃COOH and KOH from section III.A.

B. Compare the form of this equation with the equations you wrote for HCl and KOH in Sections II.A. and B.

C. Compare the amount of base necessary to react with equal amounts of the same concentration of the strong acid HCl and the weak acid CH₃COOH.

D. Compare the graphs you sketched for section II.G. and III.B. Use the features of these graphs to illustrate the similarities and differences between strong acids and weak acids in a titration.

ACID/BASE SALTS

Name

Section

Problem Statement: What are the acid and base properties of salt solutions?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/ph_meter.html and open the Acid/Base pH Simulation. Your screen should look like the figure.



This simulation contains a pH meter. You can test the pH of strong and weak acid, strong and weak base, and salt solutions of different concentrations. You will set up the conditions of each measurement using the radio buttons and slide bars and then insert the pH probes into the solution to obtain the pH of the solution.

B. In the Solutions menu, select Salt I and then select NaCl. Set the concentration of the solution at 1.00 \times 10⁻² M (use the slider bar or key in 1.00 and then the radio button). Set the volume at 100 mL (use the slider bar). Click on the Insert Probes button on the pH meter. Enter your pH data in the following table.

Solution	Concentration (M)	рН	[H+]	[он-]
NaCl (aq)	$1.00 imes 10^{-2}$			
NH ₄ NO ₃ (aq)	$1.00 imes 10^{-2}$			
NaC ₂ H ₃ O ₂ (aq)	$1.00 imes 10^{-2}$			
NH₄Cl (aq)	$1.00 imes 10^{-2}$			
Na ₂ SO ₄ (aq)	$1.00 imes 10^{-2}$			
NaCN (aq)	$1.00 imes 10^{-2}$			
NaNO ₃ (aq)	$1.00 imes 10^{-2}$			
NaF (aq)	$1.00 imes 10^{-2}$			
(NH ₄) ₂ SO ₄ (aq)	$1.00 imes 10^{-2}$			

C. Remove the probes. Measure the pH of 1.00×10^{-2} M concentrations of each of the salts in the list. Record your findings in the preceding table.

II. Data Analysis and Interpretation

A. pH is defined by the equation: $pH = -\log [H^+]$. Calculate the $[H^+]$ for each of the solutions in the table in the previous section and record your results in the table.

B. In a water solution the $[H^+]$ is related to the $[OH^-]$ by the following equation:

$$1 \times 10^{-14} = [H^+] [OH^-]$$

Use this equation to calculate the [OH⁻] for each of the solutions in the table in the previous section and record your results in the table.

Solution	Acid/Base/Neutral	lons
NaCl (aq)		
NH ₄ NO ₃ (aq)		
NaC ₂ H ₃ O ₂ (aq)		
NH ₄ Cl (aq)		
Na ₂ SO ₄ (aq)		
NaCN (aq)		
NaNO ₃ (aq)		
NaF (aq)		
(NH ₄) ₂ SO ₄ (aq)		

C. Use the information from the table in Section I.B. to identify the acid/base characteristic of each of the salts. Enter your findings in the following table.

D. Write an equation representing the reaction when NaCl is dissolved in water. What ions are present. List the ions present in each solution and record them in the preceding table.

- E. In the preceding table, circle the ion responsible for the acid/base characteristic of each solution.
- F. Write a hydrolysis equation to illustrate how salts exhibit acid base properties. Pick one acid salt and one base salt. (A hydrolysis equation is written by reacting an acid or base ion with water. A hydrogen ion is either removed from the salt and added to the water or removed from water and added to the salt to form the products.)

BUFFERS

Name

Section

Problem Statement: What are the characteristics of buffer solutions?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/ph_meter.html and http://introchem.chem.okstate. edu/DCICLA/pHbuffer20.html and open both the Acid/Base pH simulation and the Buffers simulation in separate windows. Your screen should look like the following figures.



These simulations contain pH meters. You can test the pH of solutions consisting of various combinations of acid, bases and salts. You will set up the conditions of each pH measurement using the radio buttons and then insert the pH probes into the solution to obtain the pH of the solution.

According to Brønsted-Lowry theory, an acid is a substance that donates a proton in a chemical reaction. The substance that accepts the proton is defined as a base. The products that result from such a reaction also act as proton donors and acceptors for the reverse reaction. When an acid donates a proton, the substance that results is called its conjugate. Because the conjugate of an acid acts as a base in the reverse reaction, it is called its conjugate base. In the following hypothetical reaction: HX is an acid and Y is a base, HY⁺ is an acid and X⁻ is a base for the reverse reaction, and X⁻ is the conjugate base for HX.

$$HX+Y \rightleftharpoons HY^+ + X^-$$

A buffer solution is made by combining a weak acid or weak base with its conjugate. So in the above example, you could construct a buffer solution by combining HX with X⁻. A convenient source of X⁻ could be the salt NaX. In a similar fashion, the base Y has a conjugate acid HY⁺. A buffer solution could be made from Y and the salt HYCl.

One of the characteristics of buffer solutions is that they are resistant to change in pH with additions of small amounts of strong acids or bases. This makes them useful for a number of applications in medicine and as standardized solutions.

B. Using the Acid/Base pH simulation, determine the pH of a 0.10 M solution of $HC_2H_3O_2$. (Under acid solutions, choose $HC_2H_3O_2$. Set the concentration of the solution at 10.00×10^{-2} M. Set the volume at 100 mL. Click on the Insert Probes button on the pH meter.) Enter your pH data in the following table.

Solution	Concentration (M)	рН	Acid, Base, Neutral
HC ₂ H ₃ O ₂ (aq)	0.10		
HCI (aq)	0.10		
NaCl (aq)	0.10		
NaC ₂ H ₃ O ₂ (aq)	0.10		

C. Determine the pH of a 0.10 M solution of HCl. Under salt I solutions, determine the pH of 0.10 M solutions of NaCl and NaC₂H₃O₂.

II. Data Analysis and Interpretation

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A. Classify each of the solutions you measured in the previous section as acid, base, or neutral. If a solution is an acid or base, indicate if it is strong or weak. Record your findings in the previous table.

B. Write a chemical equation that reflects the acid, base, or neutral nature of each solution.

III. Data Collection

A. Using the Buffers simulation, determine the pH of a solution made by mixing 100 mL of 20.0×10^{-2} M HCl and 100 mL of 20.0×10^{-2} M NaCl. Enter your pH data in the following table.

Solution	рН	Concentration of Acid (M)	Concentration of Salt (M)
HCI (aq) + NaCI (aq)			
$HC_2H_3O_2$ (aq) + NaCl (aq)			
$HC_2H_3O_2$ (aq) + $NaC_2H_3O_2$ (aq)			

- B. Using the Buffers simulation, determine the pH of a solution made by mixing 100 mL of 20.0×10^{-2} M HC₂H₃O₂ and 100 mL of 20.0×10^{-2} M NaCl. Enter your pH data in the preceding table.
- C. Using the Buffers simulation, determine the pH of a solution made by mixing 100 mL of 20.0×10^{-2} HC₂H₃O₂M and 100 mL of 20.0×10^{-2} M NaC₂H₃O₂. Enter your pH data in the preceding table.

IV. Data Analysis and Interpretation

A. Calculate the initial concentrations of HCl and NaCl in the solution after the acid and salt solutions are mixed together in section III.A. Enter your findings in the previous table.

B. Calculate the initial concentrations of $HC_2H_3O_2$ and NaCl in the solution when the acid and salt solutions are mixed together in section III.B. Enter your findings in the previous table.

C. Calculate the initial concentrations of $HC_2H_3O_2$ and $NaC_2H_3O_2$ in the solution when the acid and salt solutions are mixed together in section III.C. Enter your findings in the previous table.

- D. Compare the initial concentrations of the HCl solutions in sections I.B. and III.A.
- E. Compare the initial concentrations of the NaCl solutions in sections I.B. and III.A.
- F. Compare the pH of the HCl (section I.B.) and NaCl solutions to the pH of the combined solutions (section III.A.). How do you account for your findings?

G. Compare the concentrations of the HC₂H₃O₂ solutions in sections I.B. and III.A.

H. Compare the concentrations of the NaC₂H₃O₂ solutions in sections I.B. and III.A.

I. Compare the pH of the HC₂H₃O₂ and NaC₂H₃O₂ (section I.B.) solutions to the pH of the combined solutions (section III.A.). How do you account for your findings?

J. Compare the pH of the HCl/NaCl solution, HC₂H₃O₂/NaCl, and HC₂H₃O₂/NaC₂H₃O₂ solutions. How would you account for the differences and similarities?

V. Data Collection

A. Using the Acid/Base pH simulation, determine the pHs of 100 mL volumes of 1.82×10^{-5} M HCl and 3.8×10^{-5} M HC₂H₃O₂ solutions. Enter your pH data in the following table.

Solution	рН	pH after adding 1×10^{-3} mol acid	pH after adding $1 imes 10^{-3}$ mol base
$1.82 imes10^{-5}$ M in HCl (aq)			
$1.82 imes10^{-5}$ M in HCl (aq) and $1.82 imes10^{-5}$ M in NaCl (aq)	4.74	2.3	11.7
$3.8 imes10^{-5}$ M in $\mathrm{HC_2H_3O_2}$ (aq)			
$3.8 imes10^{-5}$ M in HC $_2$ H $_3$ O $_2$ (aq) and $3.8 imes10^{-5}$ M in NaCl (aq)	4.74	2.3	11.7
0.1 M in HC ₂ H ₃ O ₂ (aq) and 0.1 M in NaC ₂ H ₃ O ₂ (aq)			

B. Using the Buffers simulation, determine the pH of a solution that is 0.1 M in HC₂H₃O₂ and 0.1 M in NaC₂H₃O₂. (Add 100 mL of 20×10^{-2} M HC₂H₃O₂ to 100 mL of 20×10^{-2} M NaC₂H₃O₂.) Enter your pH data in the preceding table. Then click on the Go to Part II button and add 1.00×10^{-3} moles of HCl to the mixture. Enter your pH data in the preceding table. Finally, add 1.00×10^{-3} moles of NaOH to the original mixture. Enter your pH data in the preceding table.

VI. Data Analysis and Interpretation

A. Compare the pH of the 1.82×10^{-5} M HCl solution with the pH of the combined 1.82×10^{-5} M HCl and 1.82×10^{-5} M NaCl solution. Explain any similarities or differences that you observe.

B. Compare the pH of the 3.8×10^{-5} M in HC₂H₃O₂ solution with the pH of the combined 3.8×10^{-5} M HC₂H₃O₂ and 3.8×10^{-5} M NaCl solution. Explain any similarities or differences that you observe.

C. According to the definition in section I.A., which of the combination solutions in section V.A. is a (are) buffer(s). Explain your choice(s).

D. What would happen to the pH of a buffer solution if you changed the initial concentrations of its components? Try out your prediction and test it with the software. Record your data below.

E. List all of the buffer solutions that can be made from the acids, bases, and salts listed in Part I of the Buffer simulation.

F. The chemical equation and conditions for a hypothetical buffer solution is:

$$\label{eq:HW} \begin{array}{l} \mathrm{HW}\,(\mathrm{aq}) + \mathrm{H_2O}\,(\mathrm{l}) \ \rightleftarrows \ \mathrm{H_3O^+}(\mathrm{aq}) + \mathrm{W^-}\,(\mathrm{aq}) \\ .1\mathrm{M} \ .1\mathrm{M} \end{array}$$

The solution is made by adding the salt NaW to the weak acid HW. Use this equation and Le Châtelier's Principle to explain how a buffer resists a change in pH when an acid or base is added to it.
ACTIVITIES OF METALS

Name

Section

Problem Statement: How do metals and metal ions react?

I. Data Collection: Eight Solutions

- A. The simulation is located at http://introchem.chem.okstate.edu/DCICLA/Metal-MetalIon/home. html. Open the software and go to the opening activity. You should see a graphic that appears in part like Figure A.
- B. Hold the magnifier over each beaker and "click" to view its submicroscopic contents. Record what you see on the beakers in Figure A.



Figure A.

C. In your own words, describe why H_2O molecules are not displayed when the magnifier shows the submicroscopic contents of each beaker.

II. Data Analysis

Record the number of each species in each beaker. How are these numbers related to the formula of the compound?

III. Interpretation

A. List three characteristics that are the same for all of these solutions and three characteristics that make them different.

B. Identify the species that accounts for the color of each of the four solutions. What evidence did you use to arrive at your conclusions?

C. Predict and record in Figure B what you would expect to see with the magnifier in the other beakers.



Figure B.

IV. Data Collection: Activity One

- A. Go to Activity One in the simulation, pick one of the metals and follow the instructions to test its interaction with each of the solutions. Record your observations in Table 1 below. Describe any evidence you see for a chemical reaction. What changes do you see in the metal? What changes do you see in the solution?
- B. Repeat this process with each of the metals.

	Mg ²⁺ (aq)	Zn ²⁺ (aq)	Cu ²⁺ (aq)	Ag ⁺ (aq)
Mg(s)				
Cu(s)				
Zn(s)				
Ag(s)				

V. Data Analysis

A. Write a chemical equation and the net ionic equation for each chemical reaction you observed in IV.A. Note: If you are having difficulty writing the chemical equation and net ionic equation using the information from Table 1, you may find the following helpful. In Activity One click on Molecular Scale Reactions box and follow the directions on the new page. You will be able to watch the reaction occur at the molecular scale for whatever combination of metal and solution you have selected.



B. For each metal in Table 1 indicate the metal ions it reacted with, and for each metal ion, indicate the metals it reacted with.

In Column 2a, rank the four metal ions used in IV.A in order of reactivity as indicated. In Column 2b, rank the four metals used in IV.A in order of reactivity as indicated.



VI. Interpretation

A. How are Columns 2a and 2b in the previous section related to each other?

B. For each of the metals in Column 2b, use the reactivity data you collected (Table 1) to identify the metal ions in Column 2a that chemically reacted with it. Note the position of these reacting ions in relation with the position of those that don't react. Repeat this process for each of the metals. Summarize your findings concerning the combination of reacting metals and metal ions in Column 2a and 2b in the table below.

Metal Selected in Column 2b	Metal Ions in Column 2a that React with Metal from Column 2b	Metal Ions in Column 2a that do not react with Metal from Column 2b

Write a general statement that describes the reactivity of a metal (Column 2b) with the metal ions (Column 2a).

"Click" on the molecular scale button in the laboratory simulation Activity One to view the metal/ metal ion interactions at the molecular (submicroscopic) level.

Follow the instructions in the software. Select a combination of metal and solution that results in a reaction (Table 1). Watch the animation, then Click through the slides. Relate what you observe in this Molecular Level view with your macroscopic observation for the reaction.

Select a combination of metal and solution that does not result in a reaction (Table 1). Watch the animation and Click through the slides. Relate what you observe in this Molecular Level view with your macroscopic observation for the reaction.

C. When looking at the metal in Column 2b and the metal ion in Column 2a, the charge is not balanced. Write a balanced equation relating each metal ion (Column 2a) to its corresponding metal (Column 2b).

VII. Data Collection: Activity Two

Go to Activity Two and complete the Table below using the new set of metal/metal ions.

	Fe ²⁺ (aq)	Zn ²⁺ (aq)	Cu ²⁺ (aq)	Pb ²⁺ (aq)
Fe(s)				
Cu(s)				
Zn(s)				
Pb(s)				

Table 3

VIII. Data Analysis and Interpretation

A. Write net ionic chemical equations for the chemical reactions you observed.

B. In Column 4a, rank the four metal ions used in VII in order of reactivity as indicated. In Column 4b, rank the four metals used in VII in order of reactivity as indicated.



Table 4

IX. Data Collection: Activity Three

A. Go to Activity Three and complete the Table below, using the set of metal/metal ions taken from Activities One and Two.

	Fe ²⁺ (aq)	Pb ²⁺ (aq)	Ni ²⁺ (aq)	Sn ²⁺ (aq)
Fe(s)				
Pb(s)				
Ni(s)				
Sn(s)				

Table 5

X. Data Analysis and Conclusions

In Columns 2a/2b and Columns 4a/4b you have two ranked sets of metal and metal ions. In Activity 3 you investigated a pair of metals and metal ions from the two sets in Activities 1 and 2. Based on the reactivity of these combinations of metals and metal ions, and your responses in part VI. Interpretation (page 287), rank the eight metal ions and metals you have studied.



XI. Data Collection: Activity Four

Go to Activity 4 and follow the directions. Record your observation concerning the reaction of the five metals with HCl.

XII. Data Analysis

A. For a combination of metal and HCl that reacts, write a chemical equation that describes the reaction.

B. In Activity 4, observe the reaction of a metal and HCl at the molecular scale that you described in part A above. Watch the animation and then step through the frames and write an equation that describes what is happening to the metal and a separate equation that describes what is happening to the acid. How are these equations related to each other and to the chemical equation you wrote in section XII.A.?

XIII. Interpretation and Conclusions

A. Add the hydrogen gas/hydrogen ion combination in the correct location in the tables from section X.



- B. Use the information in Columns 7a and 7b to predict the products of the following reactions.
 - a. $\operatorname{Ag}^+(aq) + \operatorname{Ni}(s) \rightarrow$
 - b. Ni²⁺(aq)+Ag(s) \rightarrow
 - c. $\operatorname{Ag}^+(aq) + \operatorname{Sn}(s) \rightarrow$
 - d. $Mg^{2+}(aq) + Ni(s) \rightarrow$
 - e. $Mg(s) + Sn(NO_3)_2(aq) \rightarrow$
 - f. $H^+(aq) + Mg(s) \rightarrow$
 - g. $HCl(aq) + Sn(s) \rightarrow$
 - h. Fe²⁺(aq)+H₂(g) \rightarrow
 - i. $Ag^+(aq) + Mg^{2+}(aq) \rightarrow$
 - j. $H_2(g) + Cu^{2+}(aq) \rightarrow$
- C. Mental Model: Draw a picture(s) that illustrates what happens at the molecular level when Ag⁺ ion and Sn metal are mixed. In words, explain what is happening in your picture(s).

D. An unknown metal, M, not studied in this experiment, is found to react with Ag⁺ ion, Pb²⁺ ion, and Cu²⁺ ion, but not with Ni²⁺ ion, Mg²⁺ ion, or Zn²⁺ ion. Where does the unknown metal, M, appear in your activity series?

VOLTAIC CELLS

Name

Section

Problem Statement: What are the electrical properties of chemical reactions?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/voltaicCell20.html and open the Voltaic Cells Simulation. Your screen should look like the figure.



This simulation contains an apparatus for measuring the voltage generated by chemical reactions. This apparatus is called a voltaic cell. Pop-out menus will allow you to select metals (electrodes) and ionic solutions to be placed into two beakers that are connected by a salt bridge. You can then connect the metals to a voltmeter to measure the cell voltage (E°).

B. Click on the left pop-out tab for metals and select silver. Click on the left pop-out tab for solutions and select $AgNO_3$ (aq). Use the right tabs and select Cu and $Cu(NO_3)_2$ (aq). Click on the power switch of the voltage meter. Observe the action of the simulation. Use the following drawing to sketch and label what is happening and to answer the following questions.



What is the voltage (E°) generated by the chemical reaction?

What direction are the electrons flowing?

II. Data Analysis and Interpretation

- A. What happens to the electrons that are on the Ag metal electrode?
- B. What happens to the electrons that are on the Cu metal electrode?
- C. Write a net ionic equation representing what is happening in the left beaker. (This is called a half-reaction.)
- D. Write a net ionic equation representing what is happening in the right beaker. (This is called a half-reaction.)
- E. Combine the two half-reactions into a complete reaction.
- F. Determine what happens if you reverse the cell by placing the Ag/AgNO₃ system in the right beaker and the Cu/Cu(NO₃)₂ system in the left beaker. Explain what you observe.

III. Data Collection

Repeat the procedure of section I for all the combinations in the following table. Record the cell voltages for each condition. Record the direction of electron flow from electrode to electrode.

Left Cell	Right Cell	Voltage (E°)	Direction of Electrons
Ag/AgNO ₃	Cu/Cu(NO ₃) ₂		From to
Ag/AgNO ₃	Zn/Zn(NO ₃) ₂		From to
Ag/AgNO ₃	H ₂ /HCl		From to
Cu/Cu(NO ₃) ₂	Zn/Zn(NO ₃) ₂		From to
Cu/Cu(NO ₃) ₂	H ₂ /HCl		From to
Zn/Zn(NO ₃) ₂	H ₂ /HCl		From to

IV. Data Analysis and Interpretation

A. For each of the six combinations in the table in section III., write the two half-reactions that are combined to generate the overall reaction. Write the half-reaction equations to accurately represent which half-reaction gains electrons (called reduction) and which loses electrons (called oxidation). The reactions for the Ag/AgNO₃ and Cu/Cu(NO₃), are shown as an example.

$\mathrm{Cu} \rightarrow \mathrm{Cu}^{2+} (aq) + 2\mathrm{e}^{-}$	E° =	volts
$\operatorname{Ag}^{+}(aq) + 1e^{-} \to \operatorname{Ag}$	E° =	volts

B. Assume that the H_2/HCl half-reaction is assigned a voltage of 0.0 v. This means that the voltage of the other three half-reactions can be assigned relative to it. Use the information from section III to assign a voltage to each of the half-reactions in the previous section. Record the voltage in the previous section. Make sure the sum of the half-reaction voltages for each cell adds up to the cell voltages that you measured in section III.

C. Rank the four half-reactions as reductions in order from highest to lowest voltage.

V. Conclusions

- A. Does Cu²⁺ react with Ag?
- B. Does Ag⁺ react with Cu?
- C. Does Cu²⁺ react with Zn?

- D. Does Ag⁺ react with Zn?
- E. How is the sign of the voltage for an overall reaction connected to whether or not a reaction will take place?

F. Make a generalization about how you could use the ranking developed in section IV.C. to predict which combinations of half-reactions will react and which will not.

CONCENTRATION CELLS

Name

Section

Problem Statement: How does concentration affect the electrical properties of chemical reactions?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/voltaicCellEMF.html and open the Concentration Cells Simulation. Your screen should look like the figure.



This simulation contains an apparatus for measuring the voltage generated by chemical reactions. This apparatus is called a voltaic cell. Pop-out menus will allow you to select metals (electrodes) and ionic solutions to be placed into two beakers that are connected by a salt bridge. In this experiment you will be specifying the concentration of the solutions being placed in the beakers in order to study how concentration affects chemical reactions. You will then connect the metals to a voltmeter to measure the cell voltage (E°).

B. Click on the right pop-out tab for metals and select silver. Click on the right pop-out tab for solutions and select $AgNO_3$ (*aq*). Specify a concentration of 2.0 M. Use the left tabs and select Ag and AgNO₃ (*aq*) with a concentration of 2.0 M. Click on the power switch of the voltage meter. Record the cell voltage in the following table.

Trial	[AgNO₃] right half-cell	[AgNO₃] left half-cell	Voltage (E°)
1	2.0 M	2.0 M	
2	2.0 M	1.0 M	
3	2.0 M	0.1 M	
4	2.0 M	0.01 M	
5	2.0 M	0.001 M	

C. Repeat the reaction with the concentrations specified for trial 2 in the previous table and record the voltage. When the reaction has stopped, a molecular view comes available. Click on the molecular view for the left beaker and describe what is happening. Write a chemical equation for this half-reaction.

Click on the molecular view for the right beaker and describe what is happening. Write a chemical equation for this half-reaction.

D. Repeat the reaction with the concentrations specified for the remaining trials in the previous table and record the voltages.

II. Data Analysis and Interpretation

- A. Write a balanced net ionic chemical equation for the overall reaction of this voltaic cell. Specify the concentrations of the Ag⁺ in the reaction. How many electrons are transferred in the reaction per Ag⁺?
- B. On the following graph, or using a graphing program, plot the relationship between the change in concentration vs. voltage. What happens to the voltage as the concentration changes? What is the nature of this relationship? Are the changes directly proportional? (Optional: How are they related mathematically? Using a graphing program, plot the cell potential E° vs. the ratio of $[Ag^+]_{right}/[Ag^+]_{left}$. Substitute cell potential E° vs. the ratio of $[Ag^+]_{right}/[Ag^+]_{left}$ for rate vs. temperature. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line.)

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C. Optional: Use the Nerst equation to calculate the expected value for the voltage of one of the trials in section I. Compare this with the value you obtained experimentally.

 $E=E^{\circ}-.059/n \log Q$

III. Data Collection

Repeat the procedure of section I. for the copper concentration cell. Record your data in the following table.

Trial	[Cu(NO ₃) ₂] right half-cell	[Cu(NO ₃) ₂] left half-cell	Voltage (E°)
1	2.0 M	2.0 M	
2	2.0 M	1.0 M	
3	2.0 M	0.1 M	
4	2.0 M	0.01 M	
5	2.0 M	0.001 M	

IV. Data Analysis and Interpretation

A. Write a balanced net ionic chemical equation for the overall reaction of this voltaic cell. Specify the concentrations of the Cu²⁺ in the reaction. How many electrons are transferred in the reaction per Cu²⁺?

B. Compare the values you obtained for voltages for Cu²⁺ solutions with those you obtained for the Ag⁺ solutions. Explain any differences you observe.

C. On the following graph, or using a graphing program, plot the relationship between the change in concentration vs. voltage. What happens to the voltage as the concentration changes? What is the nature of this relationship? Are the changes directly proportional? (Optional: How are they related mathematically? Using a graphing program, plot the cell potenial E° vs. the ratio of $[Cu^{2+}]_{right}$ / $[Cu^{2+}]_{left}$. Substitute cell potential E° vs. the ratio of $[Cu^{2+}]_{right}$ / $[Cu^{2+}]_{left}$ for rate vs. temperature. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line.)



D. Optional: Use the Nerst equation to calculate the expected value for the voltage of one of the trials in section I. Compare this with the value you obtained experimentally.

 $E=E^{\circ}-.059/n \log Q$

ELECTROLYSIS

Name

Section

Problem Statement: How is electrical energy absorbed in a chemical reaction?

I. Data Collection

A. Go to http://introchem.chem.okstate.edu/DCICLA/electrolysis10.html and open the Electrolysis Simulation. Your screen should look like the figure.



This simulation contains an apparatus for passing an electrical current through a solution. You can control the voltage and current (in amps). You can also measure the amount of time that electricity is passed through the solution.

B. Click on the right and left pop-out menu tabs for metals and select silver for each. Click on the solutions pop-out tab and select $AgNO_3$ (*aq*). Specify a voltage 0.20 volts and a current of 0.50 amps. Set the timer for the power source at 5 minutes 00 seconds. Record the starting conditions in the following table. Click the on/off switch to begin the reaction. Record your observation as the reaction proceeds. When the time has elapsed, record your final conditions in the following table.

Trial	Mass Ag (left) Before	Mass Ag (left) After	Mass Ag (right) Before	Mass Ag (right) After	Voltage (E)	Current (amps)	Time
1	10 g		10 g		0.20 v	0.50 amps	300 sec
2	10 g		10 g		0.20 v	0.50 amps	600 sec
3	10 g		10 g		0.20 v	1.00 amps	300 sec
4	10 g		10 g		0.40 v	0.50 amps	300 sec
5	10 g		10 g		0.20 v	1.50 amps	600 sec

- C. Click on New Trial. Repeat the reaction with the conditions specified for the remaining trials in the previous table and record your data.
- D. Using the same procedures as Section B., collect data for the electrolysis of Zn in $Zn(NO_3)_2$ (*aq*) solution. Use the conditions specified in the following table. Record your data.

Trial	Mass Zn (left) Before	Mass Zn (left) After	Mass Zn (right) Before	Mass Zn (right) After	Voltage (E)	Current (amps)	Time
6	10g		10g		0.20v	0.50 amps	300 sec

II. Data Analysis and Interpretation

- A. Define *current*.
- B. Write a balanced equation for the half reaction that occurs at the Ag (right) electrode in section I.B. How many electrons are transferred in the reaction per Ag⁺?

C. Write a balanced equation for the half reaction that occurs at the Zn (right) electrode in section I.C. How many electrons are transferred in the reaction per Zn²⁺?

D. Compare the amount (moles) of Ag plated out on the right electrode in trial 1 of section I.B. with the amount (moles) of Zn plated out on the right electrode in section I.D. How do you account for this relationship?

E. Using the data from sections I.B., C., and D., what factors control the moles of substance that is produced in these reactions? Write proportionality expressions that indicate how each of these factors is related to the amount.

F. Combine the factors you identified in the previous section into a single proportionality expression. Calculate the proportionality constant (called the Faraday) for the expression. What are the units for this constant?