Kinetics

Chemistry 102*: General Chemistry II*

Post-Lab & Lab Report

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Kinetics Lab Report

Chemical Kinetics: The Hydrolysis of tert-butyl Chloride

Purposes:

To study of the rate of chemical reactions in the systems of how reactant converts to the product and how difference in reaction in the different temperature affects the rate of reaction.

The method we used is spectroscopic and titrations to perform in this experiment, by known temperature

Titration is a part of process to determine the chemical reaction will be reversed and gone back neutral state in the limiting of time. Spectroscopic used to determine to the physical method of conductance of the solution.

Prelab Questions:

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- 1.Slow
- (CH3)3C-Cl→ CH3)3C-+Cl-
- 2. fast
- CH3)3C-+H2O→ CH3)3C-OH + H+

2. Graph of In([RCl])t vs t

3. Graph 1/([RCl])t vs t

4. The purpose of adding phenolphthalein in the experiment to be an indicator of how PH change during the experiment. By adding the indicator we will know and can titrate correctly

5. NaOH will provide the source of Hydrogen Ion to give the substitute products.

Procedure

Obtaining about 60 of .25 M NaOH in isopropyl 50 water in dry beaker. Rinse twice with 3 mL portion of this solution and fill the buret completely with the solution. You have to make sure there are no bubble or Co2-. Measure out 100 mL of isopropyl 50 water in Erlenmeyer. Then add 5 drop of phenolphthalein add one ml of NAOH from the burette if it it is not turning pink you should add 1 more ml of NaOH. Add about 1 mL of tert-butyl chloride to the flask by using small graduate cylinder You have to immediately turn the clock and record the time when it turns the colorless and then repeat add more NaOH again in multiple of times. To get a time in record. Afterward you have to put in flask and heated up 50 degree Celsius with so many time. Then titrate to determine the mole of the acid.

Data& graphs

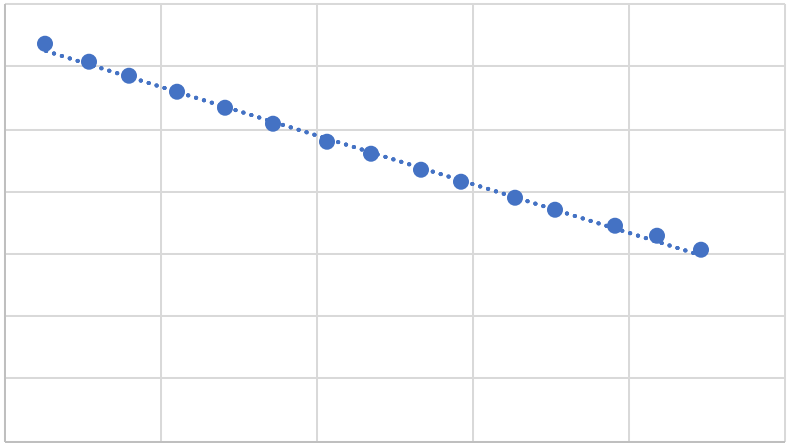
Hours Integer	Minutes Integer	Seconds integer	Total Time (s) since its inception	Initial buret reading (mL) when you filled the buret before the experiment Remember: 2 decimal places	Buret Reading (mL) Remember: 2 decimal places	Total Volume of NaOH added Remember: 2 decimal places	Molarity of NaOH from the bottle (M) Remember: 4 decimal places	Moles OH- Added (mol) Remember: proper sig. fig. w/ 3 additional digits	Total moles of RCl from Part 1 and Part 2 (mol) Remember: proper sig. fig. w/3 additional digits	$[RCl]_t$ (M) It's actually mole of RCl at time t No need to convert M	ln[RCl]t	1/[RCl] (1/M)
				0.1			0.2577		6.62E-03			
0	4	25	265		1.10	1.00		2.58E-04		0.00637	-5.057	157.104
0	9	6	546		2.20	2.10		5.41E-04		0.00608	-5.102	164.426
0	13	20	800		3.10	3.00		7.73E-04		0.00585	-5.141	170.945
0	18	25	1105		4.10	4.00		1.03E-03		0.00559	-5.186	178.823
0	23	30	1410		5.10	5.00		1.29E-03		0.00533	-5.234	187.461
0	28	43	1723		6.10	6.00		1.55E-03		0.00508	-5.283	196.977
0	34	34	2074		7.15	7.05		1.82E-03		0.00481	-5.338	208.067
0	39	5	2345		8.00	7.90		2.04E-03		0.00459	-5.385	218.003
0	44	33	2673		8.90	8.80		2.27E-03		0.00436	-5.436	229.612
0	48	43	2923		9.70	9.60		2.47E-03		0.00415	-5.485	241.021
0	54	39	3279		10.70	10.60		2.73E-03		0.00389	-5.549	256.983
0	58	50	3530		11.40	11.30		2.91E-03		0.00371	-5.596	269.475
1	5	10	3910		12.40	12.30		3.17E-03		0.00345	-5.668	289.585
1	9	48	4188		13.10	13.00		3.35E-03		0.00327	-5.722	305.546
1	14	25	4465		13.90	13.80		3.56E-03		0.00307	-5.787	326.087

Initial buret reading after 30 mins of heating (mL) **Remember: 2 decimal places**	**Final buret reading after 30 mins of heating (mL)** **Remember: 2 decimal places**	**mL NaOH added** **Remember: 2 decimal places**	**Molarity of NaOH from the bottle (M)** **Remember: 4 decimal**	**Moles OH- Added (mol)** **Remember: proper sig. fig. w/ 3 additional digits**

			places	
13.9	25.8	11.9000	0.2577	0.0031

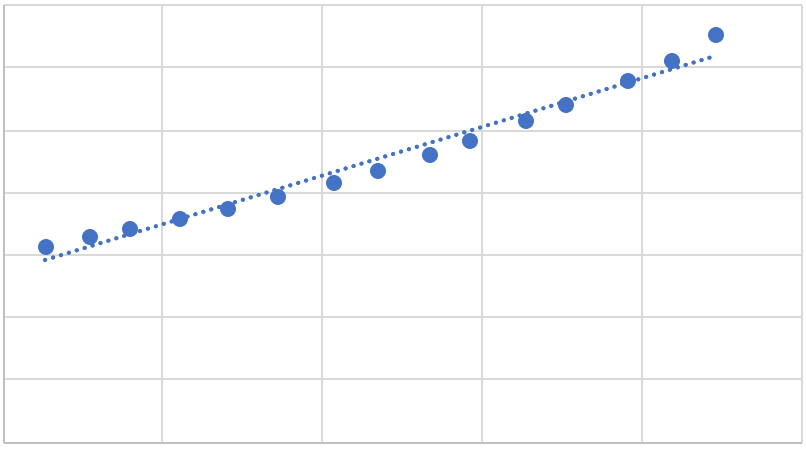
Your Summary Table				**Based on your experimentially determined reaction order, calculate the half-life and t_95% hydrolyzed. Put your answer into the appropriate boxes.**		
0th Order	**1st Order**	**2nd Order**		**0th Order**	**1st Order**	**2nd Order**
Slope Remember: 5 sig. fig	**Slope Remember: 5 sig. fig**	**Slope Remember: 5 sig. fig**		**Half-life (s) Remember: Proper sig. fig.**	**Half-life (s) Remember: Proper sig. fig.**	**Half-life (s) Remember: Proper sig. fig.**
-0.00000077619	**-0.00017103**	**0.038839**		**4163.2**	**4052.8**	**3487.2**
y-intercept, $[A]_o$ Remember: 5 sig. fig	**y-intercept, ln $[A]_o$ Remember: 5 sig. fig**	**y-intercept, 1/$[A]_o$ Remember: 5 sig. fig**		t_95% hydrolyzed (s) Remember: Proper sig. fig.	t_95% hydrolyzed (s) Remember: Proper sig. fig.	t_95% hydrolyzed (s) Remember: Proper sig. fig.
6.463E-03	**-4.996E+00**	**1.354E+02**		7910.0	17516	66257
R^2 Remember: 5 sig. fig	**R^2 Remember: 5 sig. fig**	**R^2 Remember: 5 sig. fig**				
9.977E-01	**0.99707**	**0.97653**				
Your exp. rxn order is select from the drop down menu	**0**					

Zeroth order (most linear)



First order

Second Order



Excel Calculations & Graphs

I have already calculated numbers and graphs as shown on above. The graph that are the most closely to linear is the zeroth order because it has the highest R2 value than the other graph.

Calculation

1. Based on the result of your experimental data (your reaction order), calculate the half-life for the hydrolysis of tert-butyl chloride. **[1 pt]**
2. Based on the result of your experimental data (your reaction order), calculate the time (expressed in seconds) that would have been required to hydrolyze 95% of your tert-butyl chloride if no water had been added or heating had not been employed. **[1 pt]**

Zeroth order

we could use formula from the class lecture to determine the value of half live.

$t1/2 = [A]0/2k$ --> zeroth order

$t1/2 = \ln 2/ k$ → first order

$t1/2 = 1 /k[A] 0$ k→ second order

We can find A0 from the table we makes ,then we plug in we got the solution as seconds

0th Order	**1st Order**	**2nd Order**
Half-life (s) Remember: Proper sig. fig.	**Half-life (s) Remember: Proper sig. fig.**	**Half-life (s) Remember: Proper sig. fig.**
4163.2	**4052.8**	**3487.2**

2. We used the integrate law to determine the amount of time need to be 95% hydrolyzed

$1/[A]t = kt + 1/[A]0$ → second order

$[A]t = -kt + [A]0$ --> zeroth order

$\ln[A]t = -kt + ln[A]0$ → first order

than we had .05 percent of the product left in the solution of {A}t

we can calculate then we get like

t_95% hydrolyzed (s) Remember: Proper sig. fig.	t_95% hydrolyzed (s) Remember: Proper sig. fig.	t_95% hydrolyzed (s) Remember: Proper sig. fig.
7910.0	17516	66257
.95[A]t/k=t	Ln(0.05)/-k =t	19/[A]t*k= t

Suppose that the mechanism of hydrolysis of tert-butyl chloride proceeded by a different mechanism so the predict ted rate law was: rate = k[RCl][H_2O]. From this experiment, would you be able to distinguish between a first- or second-order rate law? Explain. Hint: you may want to look up pseudo first-order reaction to help you answer this question. [1 pt]

: rate = k[RCl]'x

The actual rate is a first order reaction due to the reaction is governed by the rate determining step which includes only the tert-butyl chloride.

Since H2O does not govern the reaction and react really fast, the reaction is still dependent on [tert-butyl chloride] which shows us the reaction is a first order kinetics reaction

Conclusion:

Since we did not do the real experiment, I quite don't know what outcome to expect or errors in this reaction we can take consideration to worry and discuss about. The calculation are very simple and directed to the point we needed to complete and get it done on time.

We just did convert hour and minute to seconds by used the formula calculating the number we want to get such hour we time by 3600 and a minute by 60.

Finding the mole of NaOH from burette initial reading by using final target- initial then we can calculate mole of the certain concentration that is given M*V= mole

We derived 20^{th} row used part I and part II concentration as a mole then we use that to calculate the amount [RCl]t by using row j2 – k column then we get the answer. I used the function of ln and 1/[RCl] to calculate each of row and column then we graphed, and we did the linear fit and find the functions. The last part we did it previously.

Source of error might time taking or over titration, or the bubble from the gas on reaction, which made it inaccurate. We repeated sequence, we might over titrate then we everything will be shift and incorrect in certain ways.