**PHYSICAL CHEMISTRY LABORATORY II**

**EXPERIMENT NUMBER: 6**

**NAME OF THE EXPERIMENT: Experimental Determination of the Reaction Rate**

**DATE OF THE EXPERIMENT:27/4/2023**

**NAME OF THE ASSISTANT: Elif DEMİR ARABACI**

**GROUP NUMBER: 5**

**STUDENT NAME SURNAME: Elif Nazenin GİRAY**

**GROUP MEMBERS:Berkay Yapıcı & Alper İrez**

**SECTION: Thursday Afternoon**

**DATA SHEET**

**Table 1. Set 1 Data’s Table 2. Set 2 Data’s**

**Set 1. 50℃ K2S2O8 + KI Set 2. 25℃ K2S2O8 + KI**

|  |  |
| --- | --- |
| **Time (Sec)** | **Vtitrant** |
| **180 seconds** | **7,2 mL** |
| **420 seconds** | **11,5 mL** |
| **600 seconds** | **15 mL** |
| **900 seconds** | **16,6 mL** |
| **1200 seconds** | **17 mL** |
| **1800 seconds** | **17,9 mL** |
| **2520 seconds** | **20,4 mL** |
| **3600 seconds** | **22,4 mL** |

|  |  |
| --- | --- |
| **Time(sec)** | **Vtitrant** |
| **180 seconds** | **12,5 mL** |
| **420 seconds** | **18 mL** |
| **3600 seconds** | **19,2 mL** |

**Table 3. Set 3 Data’s**

**K2S2O8 + KI +KCl**

|  |  |
| --- | --- |
| **Time (Sec)** | **Vtitrant** |
| **180 seconds** | **9 mL** |
| **420 seconds** | **16 mL** |
| **600 seconds** | **17,8 mL** |
| **900 seconds** | **19 mL** |
| **1200 seconds** | **19,3 mL** |
| **1800 seconds** | **20,5 mL** |
| **2520 seconds** | **21 mL** |
| **3600 seconds** | **22,2 mL** |

**CALCULATION**

**Calculations for Set 2 and Set 3**

**FOR SET 2**

* Finding the concentration of S2O82- which taking from sample (from titration data)

**Reaction** : ***S2O82-(aq) + 2I.-(aq) 2SO42-(aq) + I2(aq)***

**Excess:** ***I-(aq). + (Product) I2. (aq) I3-(aq) equilibrium . I3-(aq) + Starch . Blue***

***Titration with Na2S2O3 reaction is I2(aq) + 2S2O32- , 2I- + S2O62***-

**After all I2 consumed by 2S2O32 titrant, analyte solution become colorless.**

***Titrant*** = **n(S2O32-),** = **Mtitrant x Vtitrant**

***n(I2) equal to ,*n(S2O32-)/2 and n (S2O82-)**

**M (S2O82-) =** **V=10 mL (titrated analyte)**

**[S2O82-] reacted = =>**

**[S2O82-] initial - [S2O82-] reacted = , [S2O82-] unreacted,**

**FOR SET 2 Calculation at 180 seconds,**

Mtitrant = 0.02 M; Vtitrant = 7,2 mL

[S2O82-]Reacted = [S2O82-]Initial = 0,036 M

[S2O82-]Unreacted =

Set 2 for other steps(420,600,900,1200,1800,2520,3600 seconds) applying same calculations,

**Table 4.** Unreacted concentrations with Time

|  |  |
| --- | --- |
| Time (Sec) | Unreacted Concentrations(M) |
| 180 seconds | 0,0288 |
| 420 seconds | 0,0245 |
| 600 seconds | 0,021 |
| 900 seconds | 0,0194 |
| 1200 seconds | 0,019 |
| 1800 seconds | 0,018 |
| 2520 seconds | 0,0156 |
| 3600 seconds | 0,0136 |

**2)**Plot [S2O82-]Unreacted vs time(sec) graph and fit the trend line as polynomial and choose the proper order.

**Graph 1.** [S2O82-] Unreacted vs Time (Sec) Graph

**3)**Plot the same graph [S2O82-] Unreacted vs time(sec), this time use only 3, 7, 10, 15, 20 minute data. Fit the trend line as polynomial and choose the proper order show the line equation.

**Graph 2**. [S2O82-] Unreacted vs Time(sec) for 3,7,10,15,20 minutes Graph

**4.** Take the derivative of the equation to find dc/dt.

* **From Graph 2.,**

y = (-7 ×10-14) x4 + (2x10-10 )x3 – (2x10-7 )x2 + (4x10-5)x + 0,0267 and R² = 1 thus

**At 180 seconds x equal to 0,0288 thus**

**Table 5.** Time(sec) with dc/dt values

|  |  |  |
| --- | --- | --- |
| Time(Sec) | [S2O82-] Unreacted (M) | Dc/dt (M) |
| 180 seconds | 0,0288 | 3,99885x10-5 |
| 420 seconds | 0,0245 | 3,99902x10-5 |
| 600 seconds | 0,021 | 3,99916x10-5 |
| 900 seconds | 0,0194 | 3,99922x10-5 |
| 1200 seconds | 0,019 | 3,99924x10-5 |

**Graph 3.** dc/dt (M) vs [S2O82-] Unreacted (M) Graph

**5)** Plot dc/dt vs [S2O82-] Unreacted (M) for 3, 7, 10, 15, 20min data to find the rate constant, k. in there [A] equal to [S2O82-] Unreacted thus,

d[S2O82-] Unreacted / dt = -k[S2O82-] Unreacted the slope of Graph 3 equal to negative of rate constant which is -k thus

**k=4x10-7 s-1**

**6)** Plot ln[S2O82-] Unreacted vs time(sec) for 3, 7, 10, 15, 20min data to find k.

For 180 second, ln[S2O82-] Unreacted = ln[0,0288]= -3,54738 same calculation for other time values thus,

**Table 6**. ln[S2O82-] Unreacted with time(sec) for 3, 7, 10, 15, 20min data

|  |  |  |
| --- | --- | --- |
| Time(Sec) | [S2O82-] Unreacted (M) | ln[S2O82-] Unreacted |
| 180 seconds | 0,0288 | -3,54738 |
| 420 seconds | 0,0245 | -3,7091 |
| 600 seconds | 0,021 | -3,8632 |
| 900 seconds | 0,0194 | -3,9424 |
| 1200 seconds | 0,019 | -3,9633 |

**Graph 4**. ln[S2O82-] Unreacted vs time(sec)

**6) ln[A] = ln[A]0-kt thus** ln[S2O82-] Unreacted = ln[S2O82-]0 -kt the slope of Graph 4 equal to -k ,

-k = 0,004 s-1

**7. kav ?**

(0,004+(4x10-7))/2= 2,002x10-4 s-1

**8) t1/2 ?**

**Reaction is first order reaction then** **t1/2 = ln2/k, ln2= 0,6931 k =kav**

t1/2 =(0,6931)/ 2,002x10-4 s-1 =3462,27 seconds

**FOR SET 3**

***Titrant*** = **n(S2O32-),** = **Mtitrant x Vtitrant**

***n(I2) equal to ,*n(S2O32-)/2 and n (S2O82-)**

**M (S2O82-) =** **V=10 mL (titrated analyte)**

**[S2O82-] reacted = =>**

**[S2O82-] initial - [S2O82-] reacted = , [S2O82-] unreacted**

**For set 3 at 180 seconds**

Mtitrant = 0.02 M; Vtitrant = 9 mL

[S2O82-]Reacted = [S2O82-]Initial = 0,036 M

[S2O82-]Unreacted =

Set 3 for other steps(420,600,900,1200,1800,2520,3600 seconds) applying same calculations

**Table 7.** [S2O82-]Unreacted with Time (sec) values

|  |  |
| --- | --- |
| Time (Sec) | Unreacted Concentrations(M) |
| 180 seconds | 0,027 |
| 420 seconds | 0,02 |
| 600 seconds | 0,0182 |
| 900 seconds | 0,017 |
| 1200 seconds | 0,0167 |
| 1800 seconds | 0,0155 |
| 2520 seconds | 0,015 |
| 3600 seconds | 0,0138 |

**2) Graph 5**.[ S2O82-]Unreacted  vs Time (sec) Graph

**3) Graph 6**. [S2O82-] Unreacted vs Time(sec) for 3,7,10,15,20 minutes Graph

**4)** **From Graph 6,**

y = (-4 ×10-14) x4 + (1x10-10 )x3 – (2x10-7 )x2 + (-9x10-5)x + 0,0392 and R² = 1 thus

**At 180 seconds x equal to 0,027 thus**

**Table 8.** Time(sec) with dc/dt values

|  |  |  |
| --- | --- | --- |
| Time(Sec) | [S2O82-] Unreacted (M) | Dc/dt (M) |
| 180 seconds | 0,027 | -8,9989x10-5 |
| 420 seconds | 0,0 | -8,9992x10-5 |
| 600 seconds | 0,0182 | -8,99927x10-5 |
| 900 seconds | 0,0194 | -8,99932x10-5 |
| 1200 seconds | 0,019 | -8,99933x10-5 |

**Graph 7.** dc/dt (M) vs [S2O82-] Unreacted (M) Graph

**5)** in there [A] equal to [S2O82-] Unreacted thus,

d[S2O82-] Unreacted / dt = -k[S2O82-] Unreacted the slope of Graph 7 equal to negative of rate constant which is -k thus

**k=4x10-7 s-1**

**6)** For 180 second, ln[S2O82-] Unreacted = ln[0,027]= -3,6119 same calculation for other time values thus,

**Table 9**. ln[S2O82-] Unreacted with time(sec) for 3, 7, 10, 15, 20min data

|  |  |  |
| --- | --- | --- |
| Time(Sec) | [S2O82-] Unreacted (M) | ln[S2O82-] Unreacted |
| 180 seconds | 0,0288 | -3,6119 |
| 420 seconds | 0,02 | -3,9120 |
| 600 seconds | 0,0182 | -4,0063 |
| 900 seconds | 0,017 | -4,0745 |
| 1200 seconds | 0,0167 | -4,0923 |

**Graph 8**. ln[S2O82-] Unreacted vs time(sec)

**6) ln[A] = ln[A]0-kt thus** ln[S2O82-] Unreacted = ln[S2O82-]0 -kt the slope of Graph 8 equal to -k ,

-k = 0,004 s-1

**7) kav ?**

(0,004+(4x10-7))/2= 2,002x10-4 s-1

**8) t1/2 ?**

**Reaction is first order reaction then** **t1/2 = ln2/k, ln2= 0,6931 k =kav**

t1/2 =(0,6931)/ 2,002x10-4 s-1 =3462,27 seconds

**SET 1 CALCULATIONS**

**9**) ***Titrant*** = **n(S2O32-),** = ,**Mtitrant x Vtitrant**

***n(I2) equal to ,*n(S2O32-)/2 and n (S2O82-)**

**M (S2O82-) =** **V=10 mL (titrated analyte)**

**[S2O82-] reacted = =>**

**[S2O82-] initial - [S2O82-] reacted = , [S2O82-] unreacted**

**For Set 1 at 180 seconds, Vtitrant = 12,5 mL ,** Mtitrant = 0.02 M;

[S2O82-],Reacted =

**For Set 1 at 420 seconds, Vtitrant = 18 mL, ,** Mtitrant = 0.02 M;

; [S2O82-]Reacted =

**For Set 1 at 3600 seconds, Vtitrant = 19,2 mL, ,** Mtitrant = 0.02 M;

; [S2O82-]Reacted =

***R= Δc/Δt thus,***

* For 180 seconds,
* For 420 seconds,
* For 3600 seconds,

**10.** Compare the reaction rate with 3rd min data for (set2) 25℃and (set1) 50℃,

**FOR SET 2 at 180 seconds, at 25℃**

[S2O82-],Reacted = firstly no reacted happen thus a at 0th  min 0 M thus

**FOR SET 1 at 180 seconds, at 50℃**

As the temperature increased, it was observed that the reaction rate increased, as shown in the calculations, which shows that the reaction is endothermic.

**QUESTIONS**

1. During the experiment, cold water was added to prevent the reaction from proceeding before the titration because ,theoretically, the reaction was known to be endothermic in our experiment. As a result of the ***R= Δc/Δt process*** in calculation number 10, this theory has been, proven to be correct. It is known that the temperature increase will increase the reaction rate because this is an endothermic reaction.
2. The ionic strength between the ions is expected to increase if the presence of ions ,increases, and on the other hand, if the ions have charges with the same sign, the, increasing ionic strength is expected to increase the rate constant but if the ions have different charges it will decrease the rate constant[1] .In Set2 and Set3 the effect of the increasing ion interaction on the reaction rate to examine it we added KCl to Set3 and thus increased the number of ions.,As a result of the increase in the number of ions in, the experiment and the interaction brought by it was expected that the rate constant would increase for Set3 however, in the calculations made for Set2 and Set3 in the calculation part of the report, it was observed that the reaction rate did not increase for Set3..

Product

1. aA + bB

Suppose we have a reaction above.

The formula for the rate of this reaction is with stoichiometric values,

OR

**a+b = 0 → Zero order**

**a+b=1 → First order**

**a+b=2 → Second order**

k is the rate constant and finding the order of reaction, the “a” and “b” must be summarized.[2]

* Reactants may have different concentrations in reactions. In a situation where the, order of the reaction is unknown, there may be concentrations that vary according to the rate it has.,By doing the reverse operation, we can find the reaction order by comparing the reaction rates where the changing concentrations of a reaction whose, order we do not know are equal.[2]

For instance,

aA + bB → Product

k= 1,8 x10-5  [A]= 10 M [B]= 1M => 102= 100 then order of reaction is 2.

**DISCUSSION**

To examine how the reaction rate is affected by the temperature at which the reactions take place and their ionic strengths, the solutions were discussed at different temperatures and the effectiveness of different ionic strengths in the environment., For these purposes, three sets of experiments were established for the solutions.Set1 and Set2 were appointed to investigate the effect of temperature on the reaction rate reaction used in these two sets is:

**S2O82- (aq) + 2I-(aq) →2SO42-(aq) + I2(aq)**

In Set 1, this reaction occurred at 50°C; in Set, 2, this reaction occurred at 25°C.

To examine the effect of the ionic power created by the ions on the reaction rate, the Set2 and Set3 stages were established in the experiment. The reactions in Set2 and Set3 occurred at the same temperature, but KCl was added to Set3 differently than Set2. Measurements were taken at certain times to compare the reaction rates in different conditions prepared in the experiment. Titration into solutions before applying the process, we wanted to stop the progress of the reaction with 200 mL of distilled water, because we theoretically knew that the reaction, we were working on was endothermic.

Na2S2O3 and Starch were used to titrate the solutions in the experiment. The titration process, was used to determine the concentrations of the reactants before and after the reaction. Strach was used because it decomposes in case, of excess iodine ions. Since the reaction is endothermic, the reaction rate is expected to increase as the temperature rises. As a result of the data taken from Set1 and Set2 and the calculations made afterwards, the reaction rate increased, proving the theory. On the other hand, in the calculations made for Set2 and Set3, it was not observed that the reaction rate increased despite the increasing ion effect.

Some errors may have occurred during the titration that causes to same rate constant values for Set2 and Set3. Among the main reasons, there may have been problems in the thermal equilibrium of the water bath because the lid could not be closed. Time errors may have occurred. The temperature of the environment may have affected the experiment. The volumes spent during titration may have been misread. na2so3 may have been used too much. Using more Starch than requested may have caused an error.

**References**

[1]Liu, Y., Sheaffer, R. L., & Barker, J. R. (2003). Effects of temperature and ionic strength on the rate and equilibrium constants for the reaction I•aq + i-aq ↔ I2•-aq. *The Journal of Physical Chemistry A*, *107*(48), 10296–10302. <https://doi.org/10.1021/jp036126a>

[2]Atkins, P. W., & Paula, J. D. (2014). Chapter 20 Chemical Kinetics. In *Atkins' physical chemistry* (pp. 819–878). essay, Oxford University Press.