

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

## Design

### Research Question

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

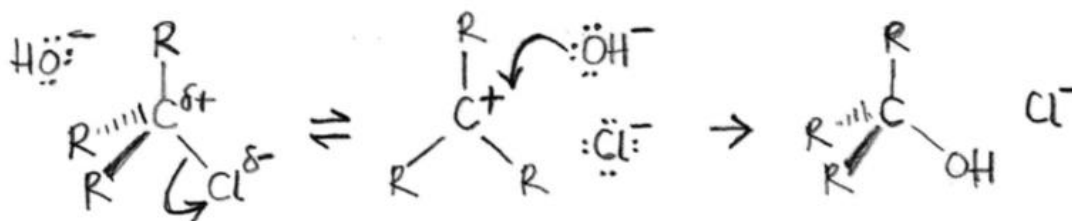
### Preliminary Discussion

When designing this experiment, the initial research question focused specifically on how the carbon-halogen bond of a halogenoalkane affects its activation energy. However, of the three primary halogenoalkanes that were in the store room: 1-iodobutane, 1-bromobutane and 1-chlorobutane - in the preliminary experiments 1-chlorobutane could not be made to react and form a precipitate despite increasing the temperature and volume of aqueous silver nitrate, meaning that it couldn't be used to explore the research question. The only other halogenoalkanes in the cupboard were tertiary, so this led the experiment to adopt the additional question about how activation energy varies depending on the type of nucleophilic substitution, while still comparing the activation energy depending on different carbon-halogen bond in primary haloalkanes, and tertiary haloalkanes.

### Background Information

The hydrolysis of halogenoalkanes occurs via a specific reaction mechanism called nucleophilic substitution. Nucleophilic substitution involves an external nucleophile (often  $\text{OH}^-$ ) reacting with an electrophile in a molecule, replacing an atom or group of atoms in the molecule.

2-bromo-2-methylpropane and 2-chloro-2-methylpropane are tertiary haloalkanes so they go through a different type of nucleophilic substitution called  $\text{S}_{\text{N}}1$ :



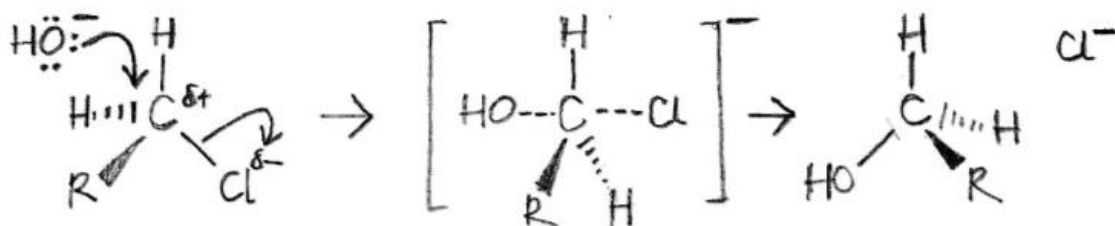
1

This is a two step mechanism, and the 1 refers to the number of species in the rate determining step. The first step is the slowest (therefore the rate determining step), and it produces a carbocation and a chloride ion. A pair of lone electrons on the  $\text{OH}^-$  (the nucleophile) will react quickly with the carbocation and substitution has then occurred, and a chloride ion is produced which can then react with silver nitrate to produce a precipitate that can be utilised to measure the activation energy for this reaction.

<sup>1</sup> Lloyd, P. StudyIB Chemistry: Types of organic reactions and synthetic routes. Retrieved June 11, 2024, from StudyIB - Your IB Learning Companion website: [Types of organic reactions and synthetic routes](#)

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1-iodobutane and 1-bromobutane are primary haloalkanes and due to this the type of nucleophilic substitution they go through is  $S_N2$ :



2

$S_N2$  is only a 1 step reaction, yet a transition state is often shown to display how one bond is breaking between the carbon and chlorine, while another one is forming between the hydroxyl and carbon. Substitution has occurred once these bonds have broken/formed, leaving a chloride ion.

In this experiment, water is the nucleophile that displaces the iodine/bromine/chlorine atom from the molecules so that it can form a precipitate with the silver (silver iodide/bromide/chloride), the rate that this precipitate forms can be utilised to figure out the activation energy of the reaction. In this experiment, the rate that the precipitate forms is judged by how quickly a black cross is obscured.

The different carbon-halogen bond strengths are listed below, this should give an early indication as to what primary haloalkane and what tertiary haloalkane have a higher activation energy than the other haloalkane that undergoes the same nucleophilic substitution reaction:

Carbon-halogen	Bond strength/ $\text{kJ mol}^{-1}$
C-I (Carbon-Iodine)	213
C-Br (Carbon-Bromine)	285
C-Cl (Carbon-Chlorine)	327

*Bond strength values<sup>3</sup>*

These values support a hypothesis that the order of activation energy of halogenoalkanes (that undergo the same type of nucleophilic substitution) will decrease as the bond strength of the carbon-halogen bond decreases.  $\text{C-I} < \text{C-Br} < \text{C-Cl}$ . The bond strength decreases as you go down group 7 (halogens) because the atomic radius increases. Therefore, the bonding electrons are further from the nucleus (causing the bond to be longer) and experience less attraction to it, meaning the bond is more easily broken.

Lastly,  $S_N2$  is an incredibly useful reaction mechanism in the pharmaceutical industry. As the nucleophile always attacks the halogen (leaving group) from the opposite side of the molecule, when it bonds at the backside of the molecule, it results in an inversion of the

<sup>2</sup> Ibid

<sup>3</sup> [www.wiredchemist.com](http://www.wiredchemist.com). (n.d.). Common Bond Energies [online] Accessed: 10/10/2024. Available at: [Common Bond Energies](http://www.wiredchemist.com) (D)

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

chirality of the optical isomer.<sup>4</sup> This means that a specific optic isomer can be isolated, ensuring that the chemical has the intended effect.

## Variables

*Independent variable when finding activation energy:* the halogenoalkane used

*Independent variable when finding the activation energy of specific halogenoalkane:* the temperature of the water bath that the solution is placed in

*Dependent variable when finding the activation energy:* time taken for the cross to disappear

*Data collection:* collected 5 temperatures for each halogenoalkane to create a gradient of activation energies that could be used to compare the haloalkanes. Tried to collect 3 values at each temperature to get a reliable mean.

Control variable	Why it was controlled	How it was controlled
Volume of aqueous silver nitrate (1.00 cm <sup>3</sup> )	To ensure that the volume of the catalyst is constant for each repeat of the experiment	Used a graduated pipette and pipette filler to accurately measure the volume of silver nitrate solution
Concentration of aqueous silver nitrate (primary - 0.100 mol dm <sup>-3</sup> ) (tertiary - 0.010 mol dm <sup>-3</sup> )	To ensure that all halogenoalkanes were reacting with the same strength of catalyst	Using premade solutions from the laboratory
Volume of ethanol (1.00cm <sup>3</sup> )	To ensure that the volume of the solvent remained constant	Used a graduated pipette and pipette filler to accurately measure the volume of ethanol
Concentration of ethanol (1.0 mol dm <sup>-3</sup> )	Used pure ethanol so there were no other reactants that could affect the rate of reaction	Using premade 100% ethanol solutions from the laboratory
Volume of halogenoalkane (primary - 2 drops) (tertiary - 1 drops)	To ensure that each test had the same volume of reactants	Used a dropper to accurately add halogenoalkane to the solution

<sup>4</sup> Chemistry LibreTexts. (2016). 11.2: The SN2 Reaction. [online] Available at: [https://chem.libretexts.org/Courses/Athabasca\\_University/Chemistry\\_350%3A\\_Organic\\_Chemistry\\_I/11%3A\\_Reactions\\_of\\_Alkyl\\_Halides-\\_Nucleophilic\\_Substitutions\\_and\\_Eliminations/11.02%3A\\_The\\_SN2\\_Reaction](https://chem.libretexts.org/Courses/Athabasca_University/Chemistry_350%3A_Organic_Chemistry_I/11%3A_Reactions_of_Alkyl_Halides-_Nucleophilic_Substitutions_and_Eliminations/11.02%3A_The_SN2_Reaction).

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

## Methodology

Risk	Precaution
The fumes from halogenoalkanes can be toxic if inhaled	Used a fume hood
Ethanol and halogenoalkanes are flammable	Used a water bath to heat up water rather than use any naked flames to heat
Silver nitrate is corrosive	Treated spillages of aqueous silver nitrate with caution and cleaned it up without skin coming into contact with it

### Environmental considerations

Some hydrocarbons, like chlorofluorocarbons, are harmful to the environment as they act as a catalyst for the breakdown of the ozone layer, therefore contributing to global warming.<sup>5</sup> However, the halogenoalkanes used in this experiment do not have this effect, so this was an environmental risk that was avoided.

However, the halogenoalkanes had to be disposed of correctly, as they can be toxic if they get into the water system and into natural environments such as ponds. Therefore, they were placed in a hydrogenated chemicals vessel for disposal.

### Ethical considerations

No ethical considerations arose during the experiment, as it didn't involve any living organisms or have any negative effects on the environment/community.

### Equipment

2 x water bath  
Fume hood  
250ml beaker (for waste)  
41 x boiling tube (40 for haloalkane solution and 1 for silver nitrate)  
Test tube rack  
Stopwatch  
Black permanent marker  
1-iodobutane  
1-bromobutane  
2-bromo-2methylpropane  
2-chloro-2-methylpropane  
Silver nitrate solution,  $0.100\text{mol dm}^{-3}$  and  $0.010\text{mol dm}^{-3}$   
Ethanol

2 x  $1.00\text{cm}^3$  pipette (one for silver nitrate solution, one for ethanol)  
Pipette filler

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<sup>5</sup> Study Mind. (n.d.). *Halogenoalkanes - Environmental Impact of Halogenalkanes (A-Level Chemistry)*. Accessed: 11/10/2024 [online] Available at: <https://studymind.co.uk/notes/environmental-impact-of-halogenalkanes/>.

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

4 x pasteur pipettes (one for each halogenoalkane)

#### **Procedure for primary haloalkanes**

1. Set water bath to desired temperature
2. Placed a test tube rack in the water bath and placed a white tile marked with a black cross (permanent marker) under one of the test tube holes
3. Filled a boiling tube with  $1.00\text{cm}^3$  of ethanol (measured using a  $1.00\text{cm}^3$  pipette and pipette filler) and 2 drops of primary haloalkane (using a pasteur pipette)
4. Filled a second boiling tube with  $1.00\text{ cm}^3$  of  $0.100\text{mol dm}^{-3}$  silver nitrate (measured using a  $1.00\text{cm}^3$  pipette and pipette filler)
5. Placed both boiling tubes in the water bath and left them to rest for 5 mins to allow solution to adjust to the temperature of the water bath
6. Placed the test tube with the ethanol + haloalkane above the cross
7. Poured the silver nitrate solution into the haloalkane + ethanol solution and started the stopwatch
8. Stopped the stopwatch once the cross was completely obscured by the white precipitate
9. Poured white precipitate into the waste beaker and put the used boiling tube into the wash. Silver nitrate boiling tube could be reused.
10. Repeated these steps 3x per temperature for each primary haloalkane and for 5 different temperatures
11. Temperatures/ $^{\circ}\text{C}$  ( $\pm 0.5$ ) used were:  
1-bromobutane: 40, 45, 50, 55, 60  
1-iodobutane: 25, 30, 35, 40, 45

#### **Procedure for tertiary haloalkanes**

1. Set water bath to desired temperature
2. Placed a test tube rack in the water bath and placed a white tile marked with a black cross (permanent marker) under one of the test tube holes
3. Filled a boiling tube with  $1.00\text{cm}^3$  of ethanol (measured using a  $1.00\text{cm}^3$  pipette and pipette filler) and 1 drop of tertiary haloalkane (using a pasteur pipette)
4. Filled a second boiling tube with  $1.00\text{ cm}^3$   $0.010\text{mol dm}^{-3}$  silver nitrate (measured using a  $1.00\text{cm}^3$  pipette and pipette filler)
5. Placed both boiling tubes in the water bath and left them to rest for 5 mins to allow solution to adjust to the temperature of the water bath
6. Placed the test tube with the ethanol + haloalkane above the cross
7. Poured the silver nitrate solution into the haloalkane + ethanol solution and started the stopwatch
8. Stopped the stopwatch once the cross was completely obscured by the white precipitate
9. Poured white precipitate into the waste beaker and put the used boiling tube into the wash. Silver nitrate boiling tube could be reused.
10. Repeated these steps 3x per temperature for each tertiary haloalkane and for 5 different temperatures
11. Temperatures/ $^{\circ}\text{C}$  ( $\pm 0.5$ ) used were:  
2-bromo-2methylpropane: room temperature, 25, 30, 35, 40  
2-chloro-2-methylpropane: room temperature, 25, 30, 35, 40

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How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

## Results

	time/s $\pm 0.25$								
temp/ $^{\circ}\text{C}$ $\pm 0.5$	Repeat 1	Repeat 2	Repeat 3	mean	Temp(K)	1/T	1/T $\times 10^{-3}$	Rate (1/time)	ln (1/t)
25.0	30.08	31.82	28.70	30.20	298	0.003355705	3.356	0.033112583	-3.408
30.0	25.58	24.33	22.05	23.99	303	0.00330033	3.300	0.041689828	-3.177
35.0	20.62	16.44	19.05	18.70	308	0.003246753	3.247	0.053466405	-2.929
40.0	10.17	11.45	11.29	10.97	313	0.003194888	3.195	0.091157703	-2.395
45.0	8.84	9.69	9.53	9.35	318	0.003144654	3.145	0.106913756	-2.236

### 1-iodobutane

Activation Energy =  $51.1 \text{ kJmol}^{-1}$  SEE **GRAPH 1** FOR PLOTTED RESULTS

### 1-bromobutane

	time/s $\pm 0.25$								
temp/ $^{\circ}\text{C}$ $\pm 0.5$	Repeat 1	Repeat 2	Repeat 3	mean	Temp(K)	1/T	1/T $\times 10^{-3}$	Rate (1/time)	ln (1/t)
40.0	460.80	567.47	527.93	518.73	313	0.003194888	3.195	0.001927773	-6.251
45.0	503.29	531.47	638.16	557.64	318	0.003144654	3.145	0.001793272	-6.324
50.0	337.47	292.12	354.78	328.12	323	0.003095975	3.096	0.003047635	-5.793
55.0	235.10	280.85	215.64	243.86	328	0.003048780	3.049	0.004100657	-5.497
60.0	187.98	175.34	177.46	180.26	333	0.003003003	3.003	0.005547542	-5.194

Activation Energy =  $64.0 \text{ kJmol}^{-1}$  SEE **GRAPH 1** FOR PLOTTED RESULTS

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

### 2-chloro-2-methylpropane

	time/s $\pm 0.25$					
temp/ $^{\circ}\text{C}$ $\pm 0.5$	Repeat 1	Temp(K)	1/T	1/T $\times 10^{-3}$	Rate (1/time)	ln (1/t)
23.0 (RT)	38.02	296	0.00337838	3.378	0.026301946	-3.638
25.0	35.77	298	0.0033557	3.356	0.027956388	-3.577
30.0	32.71	303	0.00330033	3.300	0.030571691	-3.488
35.0	24.45	308	0.00324675	3.247	0.040899796	-3.197
40.0	15.34	313	0.00319489	3.195	0.065189048	-2.730

Activation Energy =  $42.8 \text{ kJmol}^{-1}$

**SEE GRAPH 2 FOR PLOTTED RESULTS**

### 2-bromo-2-methylpropane



How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

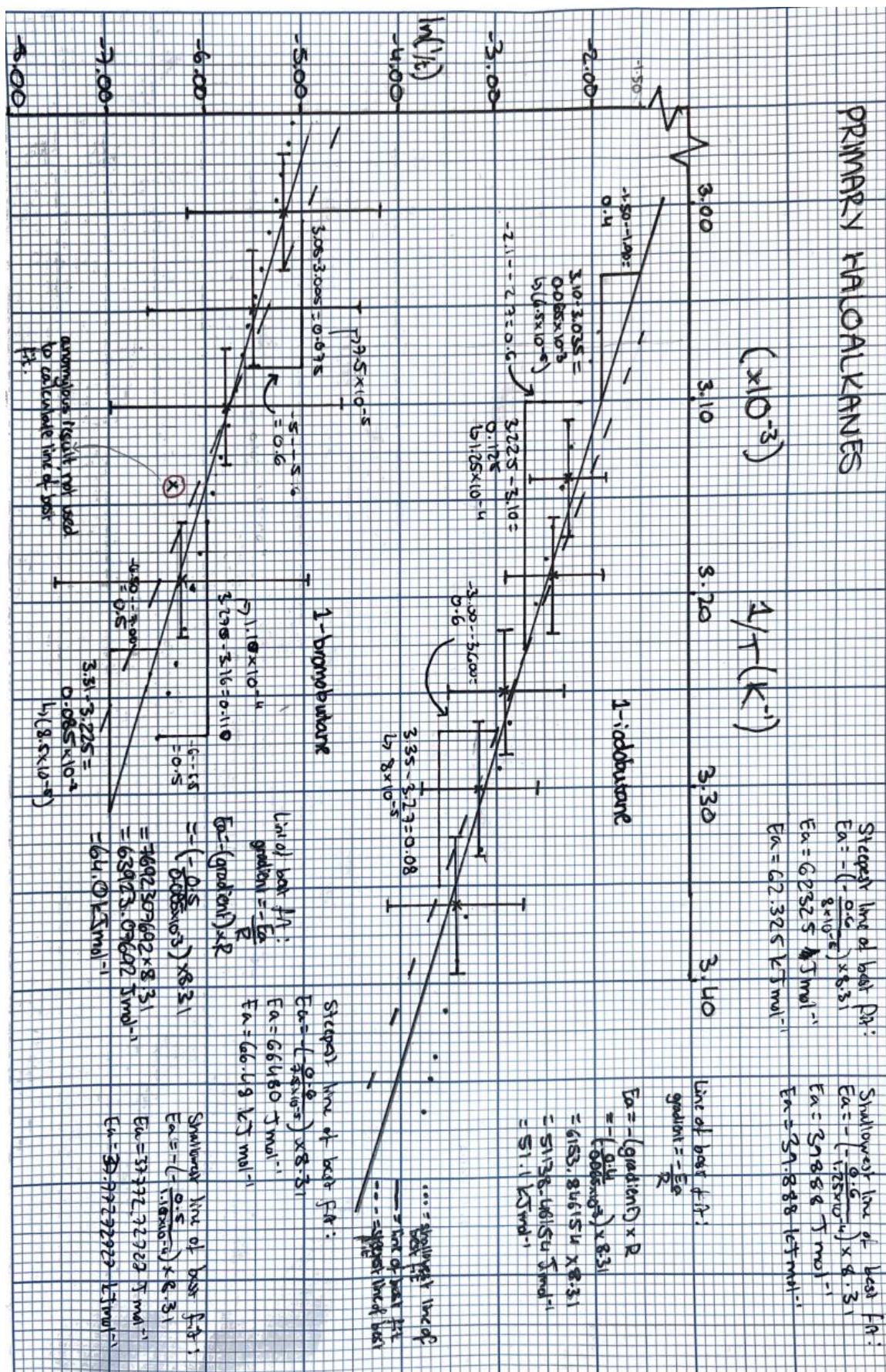
	time/s $\pm 0.25$					
temp/ $^{\circ}\text{C}$ $\pm 0.5$	Repeat 1	Temp(K)	1/T	1/T $\times 10^{-3}$	Rate (1/time)	ln (1/t)
23.0 (RT)	21.43	296	0.00337838	3.378	0.046663556	-3.065
25.0	18.96	298	0.0033557	3.356	0.052742616	-2.942
30.0	17.15	303	0.00330033	3.300	0.058309038	-2.842
35.0	15.16	308	0.00324675	3.247	0.065963061	-2.719
40.0	12.92	313	0.00319489	3.195	0.077399381	-2.559

Activation Energy =  $19.8 \text{ kJmol}^{-1}$

**SEE GRAPH 3 FOR PLOTTED RESULTS**

**Graph 1**

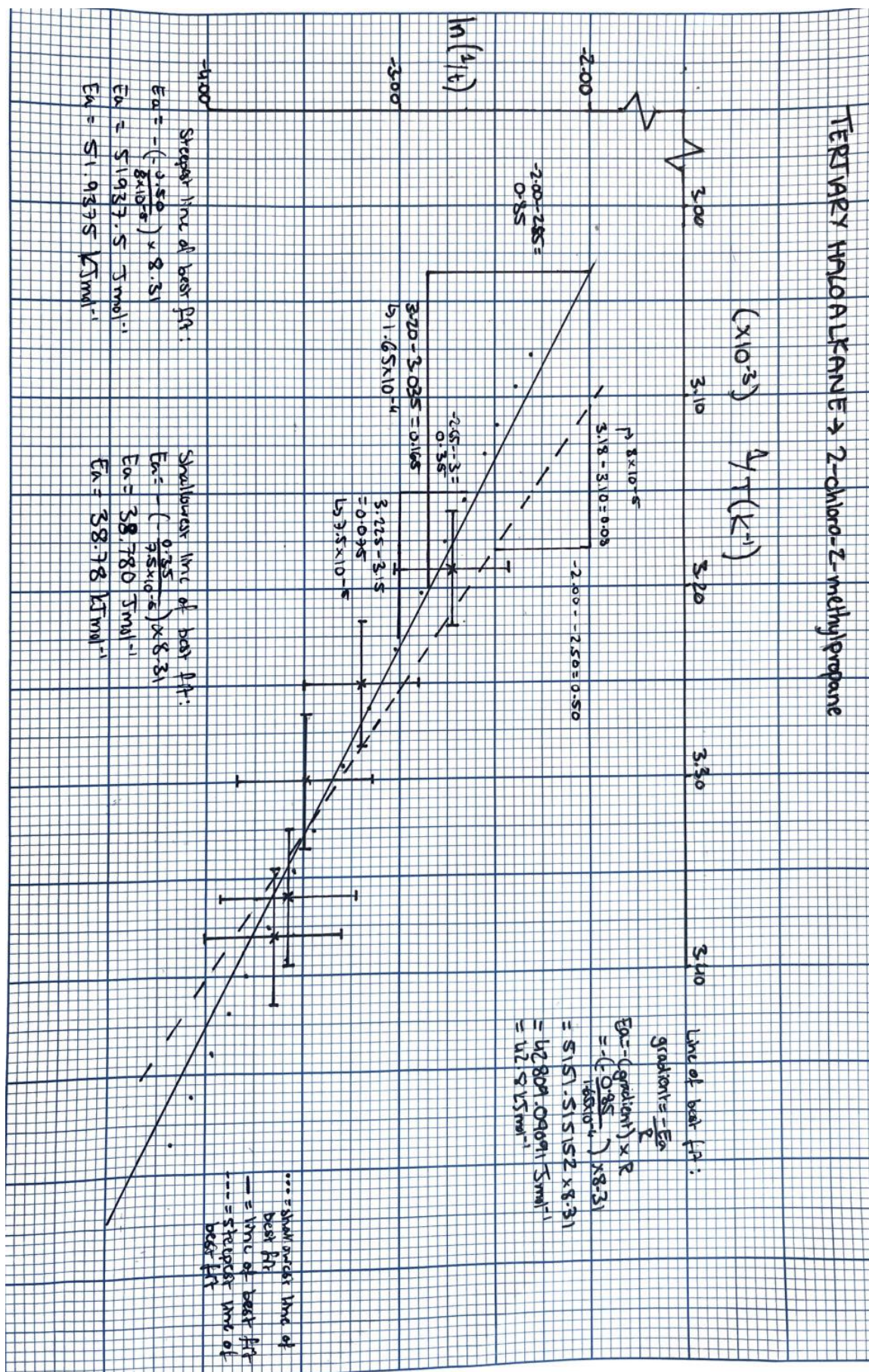
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Graph 2



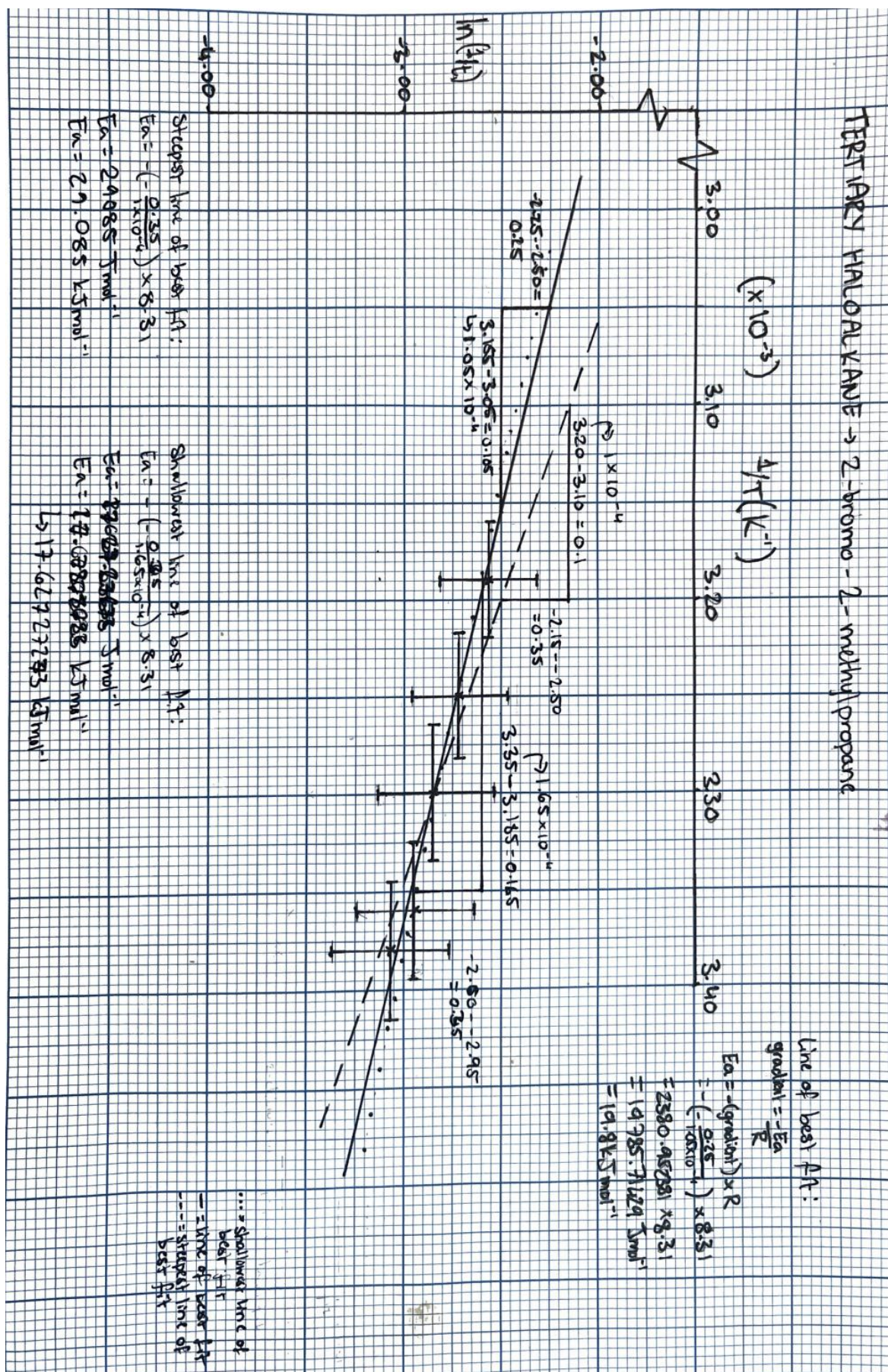
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Graph 3



How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)



Uncertainties

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

I used a 10% uncertainty for time/s. As I concluded that for every 10 seconds longer a test took to reach its end point, my area of acceptance for the end point would increase by 1 second, e.g. if a test took 40 seconds, there would be a 4 second period where the end point looked very similar to the human eye.

I used a 1% uncertainty for temperature/°C. This was a sensible average uncertainty to use for temperature. 1% came from calculating the uncertainty from a couple temperatures and it is a reasonable average to use for all temps.

30C:  $0.5/30 \times 100 = 1.667\%$

50C:  $0.5/50 \times 100 = 1\%$

70C:  $0.5/70 \times 100 = 0.7\%$

1% is a reasonable average.

Determining the uncertainty bars for x-axis on graphs is done by rounding to the nearest 0.5 on the x-axis (e.g. 3.30 round to 3.50) and then multiplying 3.50 by 0.01 (1% uncertainty for temperature) to get an uncertainty of  $0.035 \text{ } 1/T \times 10^{-3}$  to either side of the plotted point.

Then, to determine the uncertainty bars for the y-axis, I rounded the plotted point to the nearest 0.5 on the y-axis (e.g. -2.60 round to -2.50) and then multiply (-)2.50 by 0.1 (10% uncertainty for time) to get an uncertainty of  $0.25 \ln(1/t)$  to either side of the plotted point.

## Obtaining the Activation Energy from the graph results

How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

Using the Arrhenius Equation you can determine the activation energy.

$$y = mx + c \qquad \ln k = \frac{-E_a}{R} \left( \frac{1}{T} \right) + \ln A$$

6

The second equation above can be rearranged to give a straight line and used to calculate activation energy by plotting a graph of  $\ln k$  against  $1/T$ .

I have plotted  $\ln 1/\text{time}$  (proportionate to  $\ln k$ ) against  $1/\text{temp}$  so that my gradient is negative and equal to  $-E_a/R$  so that the activation energy can be calculated.

### The Arrhenius Equation:

$$k = Ae^{-E_a/RT}$$

On the graph, I calculated the gradient of my results by using the line of best fit, and then multiplied the negative reciprocal of this value by the gas constant ( $R$ ), to calculate the activation energy of the haloalkane in  $\text{J mol}^{-1}$ , however I wanted my data to be in the form  $\text{kJ mol}^{-1}$ , so I divided the answer by 1000 and rounded to the nearest 1.d.p.

### Sample calculation (for 2-chloro-2-methylpropane):

$$\text{Gradient} = -E_a/R$$

$$E_a = -(\text{gradient}) \times R$$

$$E_a = -(-0.85/0.165 \times 10^{-3}) \times 8.31$$

$$E_a = 5151.515152 \times 8.31$$

$$E_a = 42809.09091 \text{ J mol}^{-1}$$

$$E_a (\text{in kJ mol}^{-1}) = 42809.09091/1000$$

$$E_a = 42.8 \text{ kJ mol}^{-1} (1 \text{ d.p.})$$

## Table of activation energies

<sup>6</sup> Lloyd, P. StudyIB Chemistry: Types of organic reactions and synthetic routes. Retrieved June 11, 2024, from StudyIB - Your IB Learning Companion website: [Types of organic reactions and synthetic routes](#)



How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

Halogenoalkane	Activation energy (kJ/mol <sup>-1</sup> )	Minimum-maximum activation energy range (kJ/mol <sup>-1</sup> )
1-iodobutane	51.1	39.9 - 62.3
1-bromobutane	64.0	37.8 - 66.5
2-bromo-2-methylpropane	19.8	17.6 - 29.0
2-chloro-2-methylpropane	42.8	38.8 - 51.9

## Conclusion

The uncertainty ranges of the activation energies for each halogenoalkane were calculated by determining the minimum/maximum activation energy. This was done by finding the gradient of the minimum/maximum lines (which equal  $-E_a/R$ ) from the graphs, and then determining the activation energy for each of these lines.

The results show that among the haloalkanes tested, the tertiary haloalkanes had lower activation energies than the primary haloalkanes, this is easily displayed by the bromo-haloalkanes. The primary, 1-bromobutane, had a 64.0 kJmol<sup>-1</sup> activation energy, whereas this value was much lower for the tertiary, 2-bromo-2-methylpropane, with an activation energy of 19.8 kJmol<sup>-1</sup>. This reveals that primary haloalkanes require a lot more activation energy to undergo nucleophilic substitution, demonstrating that, in this case, reactions that go through the S<sub>N</sub>2 reaction mechanism require more activation energy than substances that use the S<sub>N</sub>1 reaction mechanism when they have the same carbon-halogen bond.

Furthermore, the results show how activation energy varies between halogenoalkanes that undergo the same nucleophilic substitution reaction based on the carbon-halogen bond. For the primary haloalkanes, the bromine-carbon bond (in 1-bromobutane) required more activation energy to substitute than the iodine-bond (in 1-iodobutane).

Then, the results between the tertiary haloalkanes, (2-bromo-2-methylpropane and 2-chloro-2-methylpropane), showed that during the nucleophilic substitution of these substances, the chlorine-carbon bond required more energy to substitute than the bromine-carbon bond.

This analysis correlates with the bond energies between carbon and the three halogens:

Carbon-halogen	Bond strength/kJmol <sup>-1</sup>
C-I (Carbon-Iodine)	213
C-Br (Carbon-Bromine)	285
C-Cl (Carbon-Chlorine)	327

It appears that iodo-haloalkanes require the least amount of activation energy out of the three haloalkanes tested due to having the weakest bond strength. Bromo-haloalkanes come in second, requiring more activation energy to undergo nucleophilic substitution than

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the iodo-haloalkanes, but less than the slowest haloalkanes out of the three, chloro-haloalkanes. However, to ensure that this conclusion is correct, further experiments should be carried out on 1-chlorobutane and 2-iodo-2-methylpropane to reach a fully evidenced conclusion.

## Evaluation

The most significant weakness of this experiment was that it relied upon human judgement to determine when the end point had been reached of the cross being obscured, resulting in human and random error becoming a large factor in this experiment, making it less reliable. Determining when the cross had become fully obscured, the end point of the experiment, proved difficult to identify accurately.

This became even more difficult with the less reactive substances, where the cross became obscured over a long period of time, making it almost impossible to accurately determine the same end point in each repeat. This was factored into the uncertainty for time taken for cross to obscure.

Furthermore, these results may not be repeatable by others, as a difference in eyesight can affect when someone judges that the cross has been obscured, therefore changing the results obtained from the same experiment. To overcome this obstacle of human error, a light detector could be placed below the test tube, a value for the light sensor can be decided as the end point when the timer will be stopped. This will ensure that every endpoint reached is exactly the same, and takes away any judgement having to be made by humans.

Another weakness in this experiment became apparent when I tried to get the 1-chlorobutane to react and determine its activation energy in order to draw more accurate comparisons of the significance of the type of nucleophilic substitution undergone and the carbon-halogen bond. As I was using a water bath, I couldn't get the solution hotter than 99°C which wasn't enough to get the 1-chlorobutane to react, meaning I couldn't find its activation energy. A solution to this limitation of the water bath would be to use another substance to heat the solution, such as an oil, sand or silicone bath<sup>7</sup>, which don't evaporate at 100°C like water.

When tipping the silver nitrate into the halogenoalkane/ethanol solution to begin the reaction, often the silver nitrate solution would adhere to the boiling tube surface due to how narrow it was, therefore slowing down the time for the reaction to reach its end point compared to tests where the silver nitrate solution was poured with minimal contact with the boiling tube. To solve this problem, using a funnel so the silver nitrate falls directly into the solution without touching the edges of the boiling tube could have mitigated this issue, however some may have still remained adhered to the funnel, not dropping into the solution. Another solution could be to use a wider test tube so that the silver nitrate could easily be added without coming close to the side of the test tube. However, this would make the experiment take longer as the silver precipitate wouldn't be as concentrated over the cross, resulting in it taking longer to obscure or perhaps not obscure at all if not enough silver nitrate is added. If

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<sup>7</sup> Ford, W. (2023). *How to Use a Water Bath in a Laboratory - Everything You Need To Know*. [online] VITTA Education. Available at: <https://vittaeducation.com/how-to-use-a-water-bath-in-a-laboratory-everything-you-need-to-know/>. Accessed: 14/12/2024



How does activation energy vary (determined by varying temperature and observing this effect on rate of precipitate formation) depending on the type of nucleophilic substitution and carbon-halogen bond in the hydrolysis (using aqueous silver nitrate) of different halogenoalkanes? (1-iodobutane, 1-bromobutane, 2-bromo-2-methylpropane, 2-chloro-2-methylpropane)

this solution was used, it may be best to re-evaluate the quantities of solution used in the experiment to ensure that it could still be done efficiently.

A limitation of the experiment was the lack of repeats due to the limited time to perform the experiment. This limited number of repeats decreases the accuracy of the experiment, and produces weaker data that is more susceptible to mistakes and anomalies. In an ideal environment, at least 5 repeats would have been done for each temperature of each haloalkane, this would've enabled me to correctly identify anomalies and decrease their impact on the experiment. In this experiment, it is likely that there is an anomaly with the bromobutane at 45°C, however more repeats are needed to increase this certainty as it could be that all the other results were a fluke.

Lastly, a comparison between S<sub>N</sub>1 and S<sub>N</sub>2 is partially flawed, because the rate of the S<sub>N</sub>2 substitution reaction can be affected by the strength of the nucleophile, as it is in the rate determining step. On the other hand, the nucleophile is not in the rate determining step for S<sub>N</sub>1. Therefore, this is an extraneous variable that may impact the results. It means that comparisons about the activation energy required to break the carbon-halogen bond are not as reliable when they are drawn between primary and tertiary halogenoalkanes as when they are compared between the same type of halogenoalkane.

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