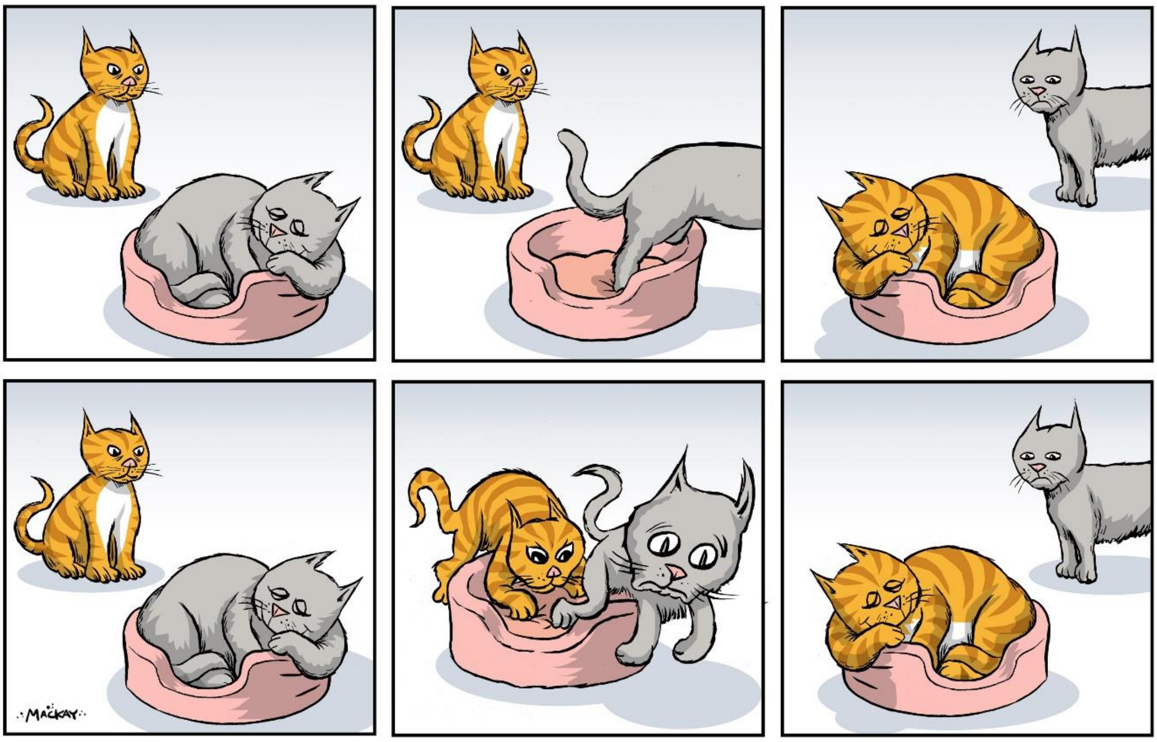
Experimental assignment P61 Class 6

(Chemistry education and research note: cohort 2 critical thinking).

Research into different reaction mechanisms in organic chemistry

Counts for 4% of the PTA.



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Take the time to read and understand the background information and assignments (+/-30 min) and check out the animations in the links, which can brighten up a lot for you.

Design and work guide of P61

We are going to do two experiments (investigations). With every experiment, you get a research question that you have to investigate experimentally. For the implementation of this research, you will make an experiment plan yourself. The PO takes 7 lessons and the schedule is as follows.

Lesson 1 and Lesson 2. Making an experiment plan for experiment 1 and 2a and 2b.

Lesson 3, Lesson 4 and Lesson 5. Performance of experiment 1, 2a and 2b

Lesson 6 and Lesson 7 Analysis of the experiments and discussion and writing a conclusion.

Rating

What do you submit and how is this assessed? For this practical assignment, you will eventually deliver both your lab journal and written report. In the lab journal, you can see the process of the development of the experiment plan and the observations and measurement values of the experiments. The lab journal, together with the notes of the teachers during the lessons , determine for 40% your grade, the report for 60%.

Use of the lab journal: During the first lessons you make in the lab journal an experiment plan with which you can examine the research question. You then use the lab journal during the execution of the experiment to write down your observations, measurement values and details about the performance of the experiment. Just before you conduct the experiment it is often useful to think about how you can conveniently note down the measured values

There are no long phrases in the lab journal. You can write it down briefly and concisely. It is a sort of experimental log. It must be easy to follow for yourself and your partner. Take the time to record your observations and measurement values during the experiment and to indicate if you change anything. Also, state why you might change something. It is very nice to have a good lab journal when you start writing the report.

Experiment plan (in the Lab journal)

- To write your experiment plan, you can use the **TIPS** that are provided with each experiment.
- *In any case, make sure that the following points are covered in the experiment plan:*
    - For each experiment, write down the ***research goal*** in your lab journal.
    - Which measurement data do you need to be able to answer the research question?
    - What is the ***independent variable*** (what do you vary yourself)? What is the dependent variable (what effect do you measure)? Which variables could influence the outcome of the experiment, but should you keep constant ("variables kept constant")?
    - How are you going to conduct the experiment and what are you going to observe/measure. (Do not just write ***that*** you are going to measure something. So for example do not just state *we are going to vary the temperature and then measure the rate of the reaction*, but think also between what values you are going to vary the temperature, every how many degrees you would like to

measure, how to make the reaction to occurs, and how to follow the course of the reaction.
  - How do you check if the measurements are ***reproducible***?
  - How are you going to ***process*** the measurement data to answer the research question? What data are you going to plot in tables and/or graphs? And what information are you going to extract from it.

- Write down the experiment plan in such a way that it is easy for someone else in the class to follow.
- Exchange the created experiment plan with 1 or 2 other groups. Write down your findings. What tips did you give other groups, and what tips did you get from the other groups? Feel free to adjust your work plan. Then write down which adjustments you have made and why.

Execution of the experiment (Note your observations/measurement values in the lab journal)

- Execute the experiment according to your work plan and write down your observations clearly.
- Find out (write down) whether you could answer the research question based on the results obtained. Do you have enough data or would you like to measure something extra? Consider if you might want to repeat, improve, adjust, or expand the experiment to obtain additional or more reliable information to answer the research question. Is there perhaps another experiment that you could carry out (with the available materials) to investigate in a different way the reaction mechanism that could confirm your findings? Write down in your lab journal what you would like to measure (in case of doubt check with the teacher what is possible) and execute this new experiment.
-

Writing a report (60%)

Write the following sections for each experiment.

Introduction Theoretical background and an introduction to the purpose of the experiment.
Materials and methods write down how you performed the experiment and, if necessary, adjusted it **(Intr. + M&M: 20%)**

Analysis of the results (20%)

Present all measurement results that you have. Analyze the results and display them on tables and/or graphs. If you have done an experiment several times then you must indicate this (even if an experiment had failed once, briefly describe it). The tables and graphs must be easy to read without consulting the text. Indicate what you can see directly in the results and what conclusions you can derive from them. Also, add all calculations done on the results in this section.

Discussion and reflection (together with conclusion / presence afterword, 20%)

Reflect on the outcome of your experiment.
You can discuss the following points:

- To what extent have you been able to answer the research question in this experiment? Evaluate the process and the results obtained (you can summarize the results here, and then put them in a broader perspective).
- On the basis of your results, what can you say about the reaction mechanism of the various reactions you have studied?

- How does the outcome of your experiment compare with what you can find in your textbook or in other sources about S_N1 and S_N2 response mechanisms?
- Do you think the measurement method was reliable? How reproducible are the measurements? What allows you to conclude that?
- Are there points that you can improve, expand on change in this study?

  Conclusion: Briefly summarize what your research has yielded and what you can conclude from it.

  Afterword: Evaluate how you feel this project went and write down what else you want to say. Can you indicate what you learned in this experiment? You can do this in one go for all experiments.

Background information to the experiment

Halogen alkanes are substances that are synthesized by chemists. Some halogen alkanes can be found naturally in certain organisms, but most halogen alkanes on earth are manufactured by chemists to be used as solvents, insecticides, fire retardants, and in the past as coolants in refrigerators (CFCs). The latter is now prohibited because CFCs contributed strongly to the development of the hole in the ozone layer. At present, the use of halogen alkanes in flame retardants is particularly a problem because they end up in the ocean and accumulate in the fat of marine animals. In this practicum, all used chemicals are collected as organic chemical waste. Halogen alkanes are very important in chemical laboratories because they are easy to convert to other compounds. One such way is nucleophilic substitution. In this practicum, we deal with different nucleophiles substitution reactions that proceed according to an S_N1 and/or an S_N2 mechanism. The principle of these two reaction mechanisms is beautifully illustrated in the cartoon on the front of this booklet. The end result of the upper and lower situation is the same. However, the reaction mechanisms of the two situations differ. In the upper situation, the red cat waits first until the gray cat has spontaneously left and takes its place as soon as the basket is empty (S_N1). In the lower position, the red cat hunts the gray cat and takes its place at the same time that the red cat leaves (S_N2).
An example of a nucleophilic substitution reaction is given below.

$$Br^- + CH_3Cl \rightarrow CH_3Br + Cl^-.$$

In the abbreviation S_N1 and S_N2, the S stands for substitution and the N stands for nucleophile. In the nucleophilic substitution, it is the free electron pair of a nucleophilic particle (so above the free electron pair of the bromide-ion), that enters into a bond with an electrophilic part of another molecule (so above the C atom of bromomethane). To make room for the bromine-ion, a group must depart from the haloalkane. We call this particle the leaving group, in the reaction above that is the chloride-ion.

But what is the difference between an S_N1 and S_N2 mechanism? The 1 in S_N1 indicates that the rate of reaction depends only on the concentration of one starting compound (i.e. the halogen-carbon compound, the electrophile). The 2 in S_N2 indicates that the reaction rate depends on the concentration of both the electrophile and the nucleophile in the reaction.

On the basis of experimental studies on the reaction kinetics of various substitution reactions, molecular models for the S_N1 or S_N2 reaction mechanism have been developed.

S_N2 reaction

The S_N2 reaction mechanism is shown schematically below (this video shows it much nicer: https://www.youtube.com/watch?v=h5xvaP6bIZI , google S_N2 University of Surrey)

Schematic representation of an Sn2 reaction.

The reaction takes place in one concerted step where both the nucleophile and the electrophile are involved. In the transition state, the central carbon atom has a coordination number of 5. The departing group can split off from this transition state.
In the energy diagram of an S_N2 substitution reaction there is therefore just one energetic barrier (transition state) (and yes that is confusing, but that 2 stands for something else 😉). Since both starting materials are involved in forming the transition state, the reaction rate depends on both the starting materials. According to the colliding particles model, both an increase in the concentration of the nucleophile and an increase in the concentration of the electrophile will lead to an increase in the reaction rate.

Image removed due to unclear copyright
Illustration of the energy diagram of an S_N2 reaction.

S_N1 reaction
The S_N1 reaction mechanism is shown schematically below (and this video shows it much nicer: https://www.youtube.com/watch?v=h5xvaP6bIZI , google SN1 University of Surrey).

With an S_N1 the reaction speed only depends on the concentration of the halogen carbon compound and the reaction rate does not depend on the concentration of the nucleophile. We can explain this on the basis of the reaction mechanism below for an S_N1 reaction.

Image removed due to unclear copyright
Schematic representation of an S_N1 reaction and illustration with connecting funnels to illustrate the rate determining step.

The S_N1 reaction takes place step by step. First, the leaving group leaves the carbon compound to yield a positively charged carbocation (a positively charged carbon atom attached to three groups) This is the speed-determining step. After this, in a much faster second step, the negatively charged nucleophile and the carbocation react with each other.

The energy diagram that fits an S_N1 reaction is shown on the left below.

Image removed due to unclear copyright
Energy diagram of an S_N1 reaction and illustration of rate determining step with conncected funnels.

The first step in which the leaving group of the carbon compound breaks free has high activation energy, this step is therefore slow. In the second step, the nucleophile enters into binding with the carbocation. This step has low activation energy and is therefore much faster than the first step. The overall reaction rate is thus determined by the slow rate of the first step where only the carbon compound participates in. You can compare this with the picture of the funnels on the right. Here the flow rate of the water is only influenced by 'the first step' ', and this thus determines the total flow rate. The rate of water flow only depends on the diameter of the first funnel. Broadening the diameter of the second and third funnel has no influence on the flow rate (overall reaction rate). Parameters that increase the rate of the second step in an S_N1 reaction, such as the concentration of the nucleophile or the strength of the nucleophile have therefore often little or no influence on the reaction rate of the total reaction.

The goal of experiment 1:
To investigate experimentally:

- The influence the concentration of 2-chloro-2-methyl propane has on the reaction rate of the substitution reaction of 2-chloro-2-methylpropane with OH^-.
- The influence the concentration of OH^- has on the reaction rate of the substitution reaction of 2-chloro-2-methylpropane with OH^-.

We will use this information to determine experimentally which reaction mechanism describes the substitution reaction of 2-chloro-2-methylpropane with OH^- best
Use the P61 method guide when creating your experimentation plan (see page 5.)

Available Materials:

- Materials for each experiment (see above)
- 0.24 M 2-chloor-2-methylpropaan in propanon (acetone), .
- Demi-water
- 0.10 M NaOH solution
- pH indicator methyl red

TIPS experiment 1:
General comments on experiment 1

- The composition of the solvent in the reaction mixture, i.e. the ratio between acetone and water, is also of very great influence on the rate of the reaction. This ratiolab jo must be kept constant in the measurement series.
- OH^- is used in the substitution reaction. As a result, the pH will drop during the experiment and the methyl red indicator will change from yellow to red/purple (see Binas table 52).
- The substance 2-chloro-2-methyl propane (2Cl2MP) also reacts with water as a nucleophile. This results in the formation of hydrochloric acid, which also reduces the pH (see figure 35 on page 183 of your book). Since in a basic environment, the formed H_3O^+ reacts immediately with the OH^- the reaction of 2C2MP with H_2O in a basic environment gives the same products as 2C2MP with OH^- and you can follow the progress of the reaction the same way. However, it is important to ensure that no 2Cl2MP comes into contact with water before you start the reaction.

- - Starting condition: The reaction works well if you make two beakers with the following composition. You can start the reaction by mixing these beakers together. The reaction time up to the tipping point of methyl red is then probably around 25 seconds.

	Bekerglas 1A:
2CL2MP (0.24 M) 3.5 mL 2Cl2MP in 140 mL acetone	2,0 mL
Acetone	2,0 mL

	Bekerglas 2A
water	20,0
Methyl red	3 drops
0,1 M NaOH	1,0 mL

- Note that the OH^- - concentration is lower than that of 2-chloro-2-methylpropane. The 2-chloro-2-methylpropane must be in excess in all reactions (otherwise the pH indicator will never change).
- The influence of the concentration of an initial substance on the reaction rate of a reaction can be determined experimentally by measuring the reaction rate as a function of the concentration of that initial substance. Of course, the concentration of the other initial substances must be constant.
  You can do this by varying the amount of one reactant in a measurement series and maintaining the amount of the other reactant(s) constant.
- The ratio acetone: water therefore remains constant in the reaction mixture. You can adjust the amount of solvent you add (acetone and water to beaker 1 and 2, respectively) to keep the total volume the same.
- Remember that a measure of the reaction rate is inversely proportional to the time it takes to convert a certain amount of substance.

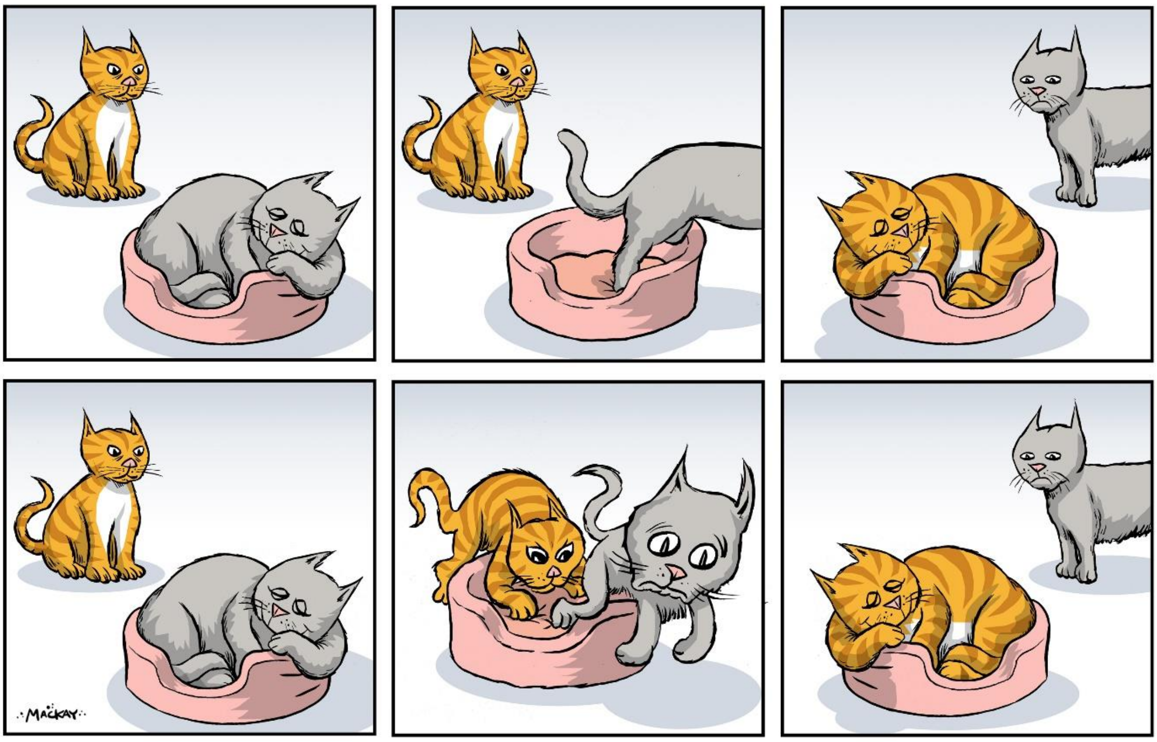
Execution of the experiment (Note your observations/measurement values in the lab journal)

- Perform the experiment according to your work plan and clearly record your observations.
- Find out (and write down) whether you could answer the research question based on the results obtained. Do you have enough data or would you like to measure something extra? Consider if you might want to repeat, improve, adjust, or expand the experiment to obtain additional or more reliable information to answer the research question. Is there perhaps another experiment that you could carry out (with the available materials) to investigate in a different way the reaction mechanism that could confirm your findings? Write down in your lab journal what you would like to measure (in case of doubt check with the teacher what is possible) and execute this new experiment.
- For the writing of the report see the guide of P61 at page 2 and further.

Experimental assignment P61 class 6 (Cohort 2).

(Chemistry education and research note: cohort 2 Paved road).

Research into various reaction mechanisms in organic chemistry



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Counts for 4% of the school exam

Take time to read through the background information and instructions and try to understand it (+/- 30 minutes). Also look at the animations in the links, which can clarify a lot.

Design and methods of P61

We are going to investigate 2 reaction series. With every reaction series, you will receive a research question that you must investigate experimentally. You follow the step-by-step plan on the next page. You are going to work with a lab journal, for which you will receive a little red notebook.

Lesson 1 and Lesson 2. Preparatory questions for Experiments 1 and 2a and 2b.
Lesson 3, Lesson 4 and Lesson 5. Execution of experiment 1 2a and 2b
Lesson 6 and Lesson 7 Analysis of the experiments and discussion and writing a conclusion.

Rating

What do you submit and how is this assessed? With this practical assignment, you submit the answers to the preparatory questions (also written in your lab journal), your lab journal and the written report.

The lab journal, together with the teacher's observations during the lessons, determine your 40% of your grade, the report 60%.

Use of the lab journal

First of all, write the answers to the preparatory questions for the experiment in the lab journal. You then use the lab journal during the execution of the experiment to write down your observations, measurement values and details about the performance of the experiment. Just before you conduct the experiment it is often useful to think about how you can conveniently note down the measured values

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Discussion and reflection (together with conclusion / presence afterword, 20%)
Reflect on the outcome of your experiment.
You can discuss the following points:

- To what extent have you been able to answer the research question in this experiment? Evaluate the process and the results obtained (you can summarize the results here, and then put them in a broader perspective).
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On the basis of experimental studies on the reaction kinetics of various substitution reactions, molecular models for the S_N1 or S_N2 reaction mechanism have been developed.

S_N2 reaction
The S_N2 reaction mechanism is shown schematically below (this video shows it much nicer: https://www.youtube.com/watch?v=h5xvaP6bIZI , google S_N2 University of Surrey)

Image removed due to unclear copyright
Schematic representation of an Sn2 reaction.

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In the energy diagram of an S_N2 substitution reaction there is therefore just one energetic barrier (transition state) (and yes that is confusing, but that 2 stands for something else 😉). Since both starting materials are involved in forming the transition state, the reaction rate depends on both the starting materials. According to the colliding particles model, both an increase in the concentration of the nucleophile and an increase in the concentration of the electrophile will lead to an increase in the reaction rate.

Image removed due to unclear copyright
Illustration of the energy diagram of an S_N2 reaction.

S_N1 reaction
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With an S_N1 the reaction speed only depends on the concentration of the halogen carbon compound and the reaction rate does not depend on the concentration of the nucleophile. We can explain this on the basis of the reaction mechanism below for an S_N1 reaction.

Image removed due to unclear copyright
Schematic representation of an S_N1 reaction.

The S_N1 reaction takes place step by step. First, the leaving group leaves the carbon compound to yield a positively charged carbocation (a positively charged carbon atom attached to three groups) This is the speed-determining step. After this, in a much faster second step, the negatively charged nucleophile and the carbocation react with each other.

The energy diagram that fits an S_N1 reaction is shown on the left below.

Image removed due to unclear copyright
Energy diagram of an S_N1 reaction and representation with connected funnels

The first step in which the leaving group of the carbon compound breaks free has high activation energy, this step is therefore slow. In the second step, the nucleophile enters into binding with the carbocation. This step has low activation energy and is therefore much faster than the first step. The overall reaction rate is thus determined by the slow rate of the first step where only the carbon compound participates in. You can compare this with the picture of the funnels on the right. Here the flow rate of the water is only influenced by 'the first step' ', and this thus determines the total flow rate. The rate of water flow only depends on the diameter of the first funnel. Broadening the diameter of the second and third funnel has no influence on the flow rate (overall reaction rate). Parameters that increase the rate of the second step in an S_N1 reaction, such as the concentration of the nucleophile or the strength of the nucleophile have therefore often little or no influence on the reaction rate of the total reaction.

General information during the experiments

Safety

The organic hydrocarbon compounds that we use are toxic and volatile. We collect these chemicals for processing as organic chemical waste. We cover supply beakers (higher concentrations) with a watch glass.

Work accurately. The reactions (especially experiment 1) that we are going to investigate are very sensitive for all kinds of influences. This means that in order to get somewhat reproducible results you have to work very precisely.

Note that your solutions do not contaminate each other. Use a separate pipette for each solution and do not swap it!! If you don't remember, grab a new one.

Make sure that you measure the quantities of the substances as accurately as possible.

Materials with every experiment

- Stopwatch (your phone, of course, you can also use it to film the experiment again 😊)
- Glass pipettes to add drops.
- Two "measuring cylinder test tubes" from the micro chem boxes to accurately add quantities of 1.0-4.0 mL.
- Beakers.

Experiment 1. Experimental research into the reaction kinetics and mechanism of the substitution reaction of 2-chloro-2-methylpropane with OH^-.

The setting of experiment 1.

Below you see both an S_N1 and an S_N2 mechanism for the substitution reaction of 2-chloro-2-methylpropane with OH^- as a nucleophile.