ARTICLE

Appendix 2

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Examining the effect of lab instructions on students' critical thinking during a chemical inquiry practical.

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Differences between cohort 1 and cohort 2

Based on the results with cohort 1, we made small adjustments to the instructions of both the paved road and the critical thinking conditions. Many cohort 1 students in the paved road group to our surprise did not compare their measurements to the S_N1 and S_N2 model for substitution reactions at all, even though these issues were clearly addressed in the pre-lab questions.

Therefore, we looked back to the Paved Road instructions. It appeared that the title above the instructions might have been misleading. The title asked the question whether the reaction was dependent on the concentration 2-chloro-2-methylpropane and OH–. Some students might have interpreted answering this question as the main research goal, and thus be satisfied with the answer that yes, the reaction rate depends on both concentrations. The instruction was reformulated to “Investigate how the reaction was dependent on both concentrations and to use this information to experimentally distinguish between an S_N1 and S_N2 mechanisms” (see student instructions in the paved road condition and below).

In the critical thinking condition of the cohort 1, the goal for the inquiry was formulated in an open way as Experimentally investigate which reaction mechanism best describes the substitution reaction of 2-chloro-2-methylpropane with OH–. With this open approach, a small fraction of students chose different approaches to investigate the reaction mechanisms, for example by changing the polarity of the solvent. In addition, some students of the cohort 1 argued that it made no sense to investigate the influence of the concentration 2-chloro-2-methylpropane on the reaction kinetics since this would have the same effect on the reaction rate in both reaction mechanisms. In the cohort 2 instructions, we wanted to focus on the students dealing with the role OH− on the observed reaction time and that the students should have a direct comparison with the effect of 2-chloro-2-methylpropane. The experimental goal in both the paved road and critical thinking assignment instruction was therefore reformulated as indicated below (also indicated in the article).

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 of the concentration of OH− has on the reaction rate of the substitution reaction of 2-chloro-2-methylpropane with OH −

Use this information to determine experimentally which reaction mechanism describes the substitution reaction of 2-chloro-2-methylpropane with OH− best.

With this more focused goal, all cohort 2 students ended up with an experimental design in which the concentration of both the reagents was varied. Since the reaction is also very sensitive to the solvent content, we added extra hints to keep the water/ acetone ratio constant for cohort 2. For future experiments, it could be a nice variation to make it more open again and to let the students have the possibility to systematically investigate the effect of the water/ acetone ratio on the reaction kinetics, as well.

In the cohort 1 study, we used disposable plastic micro reaction strips, which were changed for cohort 2 to chemical glassware because the plastic micro reaction strips were slightly affected by acetone and the shake-down technique to mix solutions by putting to two microstrips on top of each other works less well with organic solvents. The switch to glassware made the experiments easier to carry out and better reproducible for the cohort 2. Despite that with cohort 1, the experimental conditions (used chemicals and equipment) did not work out well all the time during the lessons, some students in the critical thinking condition were quite persistent to get the experiment working, whereas students in the paved road condition had

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more a wait-and-see attitude, waiting for solutions to be proposed by the teachers, or became a bit frustrated or critical. Nevertheless, the atmosphere was still very positive overall in both conditions. In the cohort 2 study, the experimental conditions had been tested better beforehand by the teachers. This resulted in fewer challenges and frustrations and a smoother course in both conditions.

Analysis of the digital questionnaire:

The magnitude of the difference between the Likert scale scores in the two conditions is analyzed by using Cohen's effect size, d, which indicates how many standard deviations the averages of the two measurements are apart and is defined by the difference between two means divided by the pooled standard deviation for the data.

For equal population size, this expression comes down to:

$$d = \frac{\mu_{CT} - \mu_{PVR}}{\sqrt{(\sigma_{CT}^2 + \sigma_{PVR}^2)/2}}$$

, in which μ_{CT} and μ_{PVR} and σ_{CT} and σ_{PVR} are the average scores and standard deviation in the critical thinking- and paved road condition.

Since the response size differed slightly between the two conditions the equation for Cohen's d value is modified to the following expression in which this is taken into account.

$$d = \frac{\mu_{CT} - \mu_{PVR}}{s}$$

with

$$s = \sqrt{\frac{((N_{PVR} - 1)\sigma_{PVR}^2 + (N_{CRT} - 1)\sigma_{CRT}^2))}{N_{PVR} + N_{CRT} - 2}}$$

In which s is the pooled standard deviation and N_{PVR} and N_{CRT} are the response numbers in the paved road and critical thinking condition, respectively ($N_{PVR} = 31$ and $N_{CRT} = 28)$. Descriptors for the magnitude of d are that the under limit for a small, medium and large and very large effect size are $d = 0{,}2$; $d = 0{,}5$; $d = 0{,}8$ and $d = 1{,}2$, respectively.

Illustrations of students argumentations in reports according to assessment rubric.

Below table 1 we give examples of students answers assigned to different level of critical thinking depicted in table 1 (also present in the manuscript).

Table 1. Assessment rubric critical thinking level. Checkpoints for identification critical thinking level in students' reports. (Also present in the article).

Level 0	No thoughtful comparison between data and models.
Level 1	A comparison between experimental data and kinetic models without realizing the real meaning of the data. E.g., interpretation of increased reaction time as a decrease of the reaction rate and the notion that a decreased reaction rate upon increased [OH^-] does not match with any of the two suggested kinetic models.
Level 2	Interpretation of the experimental data and determination of the extent to which the data correspond to the theoretical model/hypothesis. E.g., the notion that the trend in the (reciprocal of the) reaction time is not a direct measure of the reaction rate since more OH^- has to react before the pH indicator changes color.
Level 3	Quantitative interpretation of the experimental data, and of the extent to which the data correspond to the theoretical model/hypothesis. E.g., a quantitative approach of the experimental data by which the dependence of the reaction rate on [OH^-] can be evaluated.

Examples of student answers assigned to different levels of critical thinking.

(*G*oogle) Translatated fragments from students answers (with minor adjustment of the translation by the authors). Some of the formulation problems were also present in the original Dutch version and have not been repaired.

Level 0:

- The rate of the 2Cl2MP reaction with OH^- is in any case dependent on the OH^- concentration (*authors note: no notice of the sign of the influence).* According to the top graph, it seems that the 2Cl2MP concentration has no influence on the reaction rate, but that cannot be said with certainty. We think the results are reliable. It is important that careful attention is paid to ensuring that the correct number of drops (the cohort 1 condition) ends up in the containers, which can sometimes be difficult. We think we have answered the research question, since it is an S_N1 reaction, it makes sense that only 1 substance has an effect on the reaction rate.

- What the above tables show is that if NaOH is doubled, *it takes longer until a color change takes place. The reaction proceeds more slowly with more NaOH.* It also follows from the tables that if 2CL2MP is doubled, it takes less time until a color change takes place. The reaction is faster with more 2CL2MP. Does an S_N1 reaction or an S_N2 reaction better describe the substitution reaction of 2-chloro-2-methylpropane with OH-? Our hypothesis is correct. An S_N1 response best describes the substitution reaction. The concentration of OH- has *no influence* on the reaction rate, but the concentration of 2-chloro-2-methylpropane does. As the concentration thereof increases, the reaction proceeds faster. So there is only one substance that determines the reaction rate. (Note by the authors: Students contradict themselves and do not give a sign that they have thought about what makes the reaction time to become longer.)
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Level 1

- First of all, it was clear from series 1 that there is a relation between the rate of the reaction and the concentration at which the reaction proceeds faster when the concentration of 2-chloro-2-methylpropane is higher. These results are in line with what we expected after reading the book about S_N1 reaction. Namely, that with a higher concentration of this initial substance, the reaction rate becomes greater. Furthermore, the results of experiment 1 series 2 on the other hand were unexpected since the book stated that the concentration of the nucleophile would have no influence on the course of an S_N1 reaction. From our measurement results, however, there appeared to be a negative relationship between the number of mL of NaOH and the reaction time. We cannot explain this, because if the concentration of both the starting material and the nucleophile had an influence on the reaction rate, you could assume an S_N2 reaction, but with an S_N2 reaction, an increased concentration of the nucleophile would rate up the reaction and not delay it.
- The purpose of this experiment was to see if we could determine which reaction mechanism best describes the substitution reaction of 2-chloro-2-methylpropane with OH-. The results showed that when we varied the concentration of 2-chloro-2-methylpropane, the reaction time also changed. The conclusion that can be drawn from this is that the reaction time (and therefore the reaction rate) is dependent on the concentration of 2-chloro-2-methylpropane. Namely, the more 2-chloro-2-methylpropane was present, the faster the reaction proceeded. In series 2 of this experiment we did not vary the concentration of 2-chloro-2-methylpropane, but the concentration of OH-. From the results of this experiment it followed that the more OH- was present, the slower the reaction proceeded. So we can speak of an influence in series 2, but of a negative one. So we can get the following from this experiment:
  - The reaction rate is influenced by the concentration of 2-chloro-2-methylpropane
  - The reaction rate is influenced by the OH- concentration.

  We can therefore conclude from this that the reaction rate depends on two different starting substances, which indicates a Sn2 reaction. However, what is true is that the reaction time increases as more OH- is added. According to the theory behind a Sn2 reaction, with a higher concentration of one of the starting substances of the reaction, the reaction rate should increase and not decrease. In any case, the entire reaction actually refers more to a Sn1 reaction than to a Sn2 reaction. The reason for this is that 2-chloro-2-methylpropane forms a tertiary carbocation (for further information, see the "introduction to experiment 2" section) and a tertiary carbocation is very stable, which increases the reaction rate. There is also considerable spatial hindrance with the central C atom, which means that we can almost certainly say that we are talking about a S_N1 reaction.
- In experiment 1B we varied the concentration of the nucleophile, OH-, for the different measurement series. As this was added more, the reaction time became increasingly higher. This is a strange phenomenon, since the fact that if the reaction rate of the electrophile and the nucleophile both influence the reaction rate, it would be self-evident that this reaction would proceed faster as more of the nucleophile was added. However, this is not the case. It is possible that a certain error during the measurement affected the results, and the concentration of OH- would not affect the reaction rate. If this is the case, the substitution reaction of experiment 1 would be a Sn1 reaction. However, it is strange that the results are convincing enough to say that the OH- concentration does indeed have an influence on the reaction rate. In this case, both the nucleophile and the electrophile affect the reaction rate, indicating a Sn2 reaction. It is unclear why OH- has an opposite effect on the reaction rate than what we expected: 2-chloro-2-methylpropane is a tertiary carbocation. During the substitution reaction, the leaving group was a weak base. The reaction also

took place in a polar solvent showing that experiment 1 was an S_N1 reaction. In this case, therefore, a measurement error must have been made in experiment 1B and the results should have been such that the concentration of OH- had no influence on the reaction rate.

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Level 2

- …..In the second series we saw that the more sodiumhydroxide we added, the longer it took before we had a color change. This is because we have more OH- in our mixture, which means that the pH value of our mixture is higher and therefore more H + must occur until we reach the pH value for the color change of methyl red. The reaction rate has thus not decreased, but the starting point of the pH value of the mixture is therefore higher.
  ….With series 2 it was thus actually to be expected that the time until the color change became longer and longer the more NaOH we added. This is because we start with a higher pH value while the reaction rate remains the same. It is therefore not the case that the reaction rate is lower, but that the starting point is further away from the target in terms of pH value.
- Our results from series 1 have shown that the concentration of 2-chloro-2-methylpropane has an influence on the substitution reaction. You can conclude that as the amount of 2-chloro-2-methylpropane increases, the reaction time decreases, which means that the reaction rate will increase. This is the case with a Sn1 and a Sn2 reaction. Therefore you cannot conclude in the first series of experiment 1 whether it is a Sn1 or a Sn2 reaction. The results from series 2 show that as the amount of NaOH increases, the total reaction time increases, which means that the reaction rate decreases. If you increased the concentration of OH, you would expect that with a Sn2 reaction the reaction rate increases, because the OH particle is part of the speed-determining step, but this is not the case. Methyl red is used as an indicator, which means that it takes longer for all the OH to disappear, so the reaction rate ultimately remains the same.
  …….We can therefore conclude from our results that we are dealing with a Sn1 reaction.

Level 3

- (after calculating correctly (average) chemical rate values and plotting these in graphs) ……. The results of experiment 1.2 are ultimately decisive for whether it concerns an S_N1 or an S_N2. If a higher concentration of hydroxide ions were to cause a higher reaction rate, this would be an S_N2 reaction. This turned out not to be the case. The reaction rate remains approximately the same during the measurements, so that it could be concluded that it is an S_N1 reaction.
- ….The reaction mechanism that is better applicable is an S_N1 reaction. It can be concluded from the results of experiment 1 that with an increase in the concentration of 2-chloro-2-methylpropane the reaction rate increases. The concentration of 2Cl2MP therefore certainly has an influence. However *(as can be seen in the graph),* with an increase in the OH-concentration, the reaction time decreases. This is because more OH- must be converted to reach the turning point. However, if there is twice as much OH-, the reaction takes a little more than twice as long. The concentration of OH- therefore still has a negative influence on the reaction rate, because the conversion is becoming slower. This is perhaps due to the fact that the 2Cl2MP excess is getting smaller during the cause of reaction and this results in that the reaction rate is reduced (because 2Cl2MP does influence the reaction rate).