

Article

Using Stop Motion Animations to Activate and Analyze High School Students' Intuitive Resources about Reaction Mechanisms

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Abstract: Mechanisms are part of the high school curriculum in many countries. Although research shows that university students struggle with mechanistic reasoning, very little is known about learning mechanisms in high school. Understanding the cognitive resources that high school students intuitively activate is critical to fostering meaningful learning. A readily available tool for modeling dynamic processes are stop-motion animations (SMAs). In this study, 55 high school students were asked to create SMAs of their intuitive ideas of nucleophilic substitution reactions. In a second step, the students evaluated two pre-made SMAs modeling the textbook-based stepwise (S_N1) and concerted (S_N2) mechanisms. Within the student-generated SMAs, S_N1 - and S_N2 -like mechanisms were equally distributed; after viewing the textbook-style animations, most students rated an S_N2 mechanism as more likely. However, no group modeled both types of mechanisms or reasoned that both mechanisms were possible. Students used diverse chemical concepts as well as plausibility in their reasoning. However, simultaneous movement of atoms, conformational changes, and the idea of competing and boundary mechanisms do not seem intuitive. In conclusion, SMAs were found to be an appropriate tool for activating, analyzing, and discussing students' resources "on the fly", and these ideas can serve as a starting point for promoting productive mechanistic reasoning.

Keywords: reaction mechanisms; organic chemistry; stop-motion animations; resources framework; student conceptions; nucleophilic substitution; high school chemistry

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1. Introduction

Reaction mechanisms are a central tool for the description and study of organic chemical processes. They are also part of many organic chemistry (OC) curricula in high schools and universities. When students learn about reaction mechanisms, they already have a multitude of diverse ideas, concepts, and experiences, e.g., from former chemistry lessons, everyday life, or media. As proposed by Hammer et al. [1], the term 'resources' can be used as an umbrella term for these ideas. This study investigates which resources high school students intuitively activate if they are asked to reason about nucleophilic substitution reactions. Stop-motion animations (SMAs) will be used as a central tool for the analysis of students' ideas.

1.1. Reaction Mechanisms in Organic Chemistry and of the Nucleophilic Substitution

Mechanistic studies are a central part of OC. They focus on "everything which happens between reactants and products" [2], i.e., they focus on reaction processes rather than exclusively on products. This process orientation was central to the establishment of OC as a science [3]. In 1835, Friedrich Wöhler, one of the founding fathers of OC, described OC as a "jungle of the tropes, filled with the most mysterious things, ..." [4] (p. 604, translated by the author). With the advent of physical-organic chemistry [5], concepts such as electro- and

nucleophiles were established, which could serve as signposts and reaction mechanisms as paths through the wilderness. This allowed the targeted synthesis of even the most complex molecules [6].

One of the first mechanisms to be studied in detail was the nucleophilic substitution reaction. The insights gained for this reaction type played a crucial role in the development of the foundations of physical-organic chemistry [5]. Until the 1930s, in OC a “singularity of mechanisms” was assumed [7]. Thus, reaction processes were of little interest to researchers, who expected that each reaction would proceed along similar pathways. However, Ingold’s group of chemists observed that structurally very different compounds showed large differences in reactivity towards nucleophilic substitution reactions [8,9]. Kinetic measurements played a key role in these investigations [10]. To explain these observations, Ingold and coworkers proposed two distinct reaction mechanisms for nucleophilic substitution reactions: In reaction pathway I (later called S_N1 , Figure 1 top), first the leaving group (here: Br^-) is abstracted from the reactant; a cation is formed. Only *thereafter* does the nucleophile (here: Nu^-) attack the ion and form the product. In the other reaction path (later called S_N2 , Figure 1 bottom), the attack of the nucleophile and the abstraction of the leaving group happen *at the same time* [8,11].

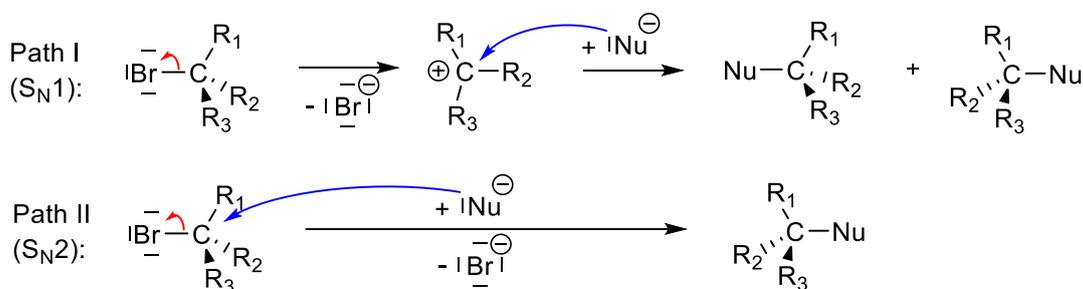


Figure 1. Schemes of the two-step (**top**) and one-step (**bottom**) reaction paths for the nucleophilic substitution for the example of a bromoalkene. R_1 – R_3 describe organic moieties, Nu an anionic nucleophile (e.g., an alkoxide).

The prominent role of nucleophilic substitution reactions in the history of science [6] highlights their potential to introduce fundamental ideas on processes in chemical reactions in high school or undergraduate chemistry [12–14].

1.2. Reaction Mechanisms in Chemistry Education

Reaction mechanisms have been included into several high school curricula, e.g., in the guidelines of the American Chemical Society [15], in France [16] or in the United Kingdom [17]. In Germany, reaction mechanisms have been part of high school curricula for many years [18], before they started to disappear from the curricula of each federal state during the last decades [19]. In 2020, reaction mechanisms were redefined as a central aspect of high school chemistry in the mandatory nationwide curriculum (“Bildungsstandards”) [20,21]. Therefore, this study investigates learning reaction mechanisms at the high school level.

Most empirical research focuses on learning reaction mechanisms at the university level [22]. These results suggest that university students often do not see reaction mechanisms as a helpful tool for understanding chemistry. In contrast, even the purpose of reaction mechanisms seems to be unclear to many students [23]. Many of them focus on specific surface features of reactants or products rather than on the overall picture of a reaction [22]. Therefore, the reproduction of mechanisms is often based on instrumental learning [23], a trial-and-error method to get to the product [24], or a focus on terminology and symbols without further understanding of the words used [25]. This is particularly evident in the case of curved arrows, which are often used as additional “decoration” of the mechanism rather than as an aid to understanding mechanisms [24–27]. As a result,

students often remain at the surface level of the “iceberg” called OC [28]. Unfortunately, this shortcoming does not allow many students to gain a deeper understanding of *mechanistic thinking*, the question of the why and how of chemical reactions [29,30]. This type of mechanistic thinking helps to translate phenomena on the macroscopic scale into processes at the sub-microscopic level [31,32].

However, the way in which OC is taught influences the extent to which students are able to use mechanistic thinking productively. For example, a focus on explaining phenomena in assessments [33], or the use of scaffolds [34], may promote a deeper understanding of reaction mechanisms. One crucial prerequisite for this kind of learning is the activation of prior knowledge, e.g., from general chemistry or other contexts [35]. This is in line with constructivist learning theories suggesting that new knowledge has to be connected with prior knowledge [36]. Thus, meaningful teaching of reaction mechanisms requires knowledge of students’ initial conceptions of reaction processes.

In general, high school students have significantly less prior knowledge in chemistry than university students. Therefore, it is very unlikely that high school students intuitively hold a coherent concept of reaction mechanisms. Nevertheless, they have a variety of different ideas or knowledge pieces from previous chemistry instruction or everyday logic [37] that they may use to reason on reaction mechanisms. The way students’ prior knowledge is organized can be understood in very different ways [38]. The next chapter gives a very brief overview of the underlying understanding of students’ mental resources, which forms the basis of the study herein.

1.3. Activation of Student Mental Resources and Learning

For decades, a large body of research has analyzed students’ (mis-)conceptions in various areas of chemistry [38,39]. Much of this research shared the same implicit assumption: Students would hold a somewhat coherent concept of chemical ideas that differed in its content but not in its structure from the correct scientific concept. In contrast, more recent psychological theories of learning suggest that it is in fact the structure of students’ knowledge that differs dramatically from that of experts [1,38,40]. Hence, the focus shifts to the following question: How is this prior knowledge of students organized? DiSessa [38] argues that students have a network of loosely organized ideas. This kind of intuitive knowledge is very difficult to describe because it comes from a wide variety of sources, such as prior learning, everyday experiences, or the media [37]. Thus, some of these mental structures are organized in a quasi-coherent network, while other parts are more like isolated ideas. When students learn or have to solve problems, they activate several of these resources. However, the context of the problem and situation determines which “resources” are activated, as Hammer et al. [1] point out. This point of view can be very helpful for teaching chemistry [41,42]. It shows that even scientifically incorrect ideas of students can be used as a starting point for learning. However, it also challenges practitioners to analyze the ideas that specific students activate in a specific situation to solve a specific problem. From the perspective described, it does not seem useful to refer to “the one” concept that students hold. Rather, it is necessary to analyze the multitude of resources students activate in the context of a specific problem. As SMA may be a useful tool for this purpose, the next chapter provides a brief overview of SMAs.

1.4. Stop Motion Animations as a Tool for Science Education

SMAs generally describe a series of images that are played at a high speed to give the impression of motion [43]. Most students will be familiar with stop-motion technique from popular TV shows such as “Shaun the Sheep” or “Wallace and Grommit” [44]. These TV shows and others use photos of plasticine models to create such animations. In general, 20–25 slightly modified frames per second are used in professional SMAs to give the impression of moving objects [43]. Even short movies require a very large number of frames, which makes the production of such SMAs time consuming. This makes it difficult to create SMAs in a school environment. In addition, for educational purposes, the fast

change of frames can be critical, as it becomes difficult to distinguish the individual movements in the frames. Therefore, Hoban [43,45] invented the term “Slowmation” which describes simplified animations with only two frames per second. Hoban and Nielsen [45,46] showed that the generation of such slowmations can help students, for example, to reflect and deepen their understanding of certain concepts. In a recent review, Farrokhnia et al. [47] provide a thorough overview of the use of student-generated SMAs in science. Most of the studies described in their review focus on student teachers, while only 14% of the studies were conducted in schools and barely 10% had a focus on chemistry education. Nevertheless, SMAs can also be helpful when students have little or no pre-knowledge of a particular area [45,47]. Consequently, SMAs have been used to analyze student perspectives. Orraryd et al. [48,49] used student-generated SMAs to foster learners’ conceptions of *evolution through natural selection*. They concluded that SMAs may be a new way of looking at students’ preconceptions because dynamic processes are easily representable. In addition, students need to reflect on the models and the different levels of representation.

The use of mental models and the dynamic representation of reaction processes are among the most important features of learning reaction mechanisms [50]. Animations or simulations are broadly used to teach reaction processes [51–54]. In most cases, such animations are only presented to students, but not created by them, because the generation is tedious and requires significant prior knowledge in programming or animating. Therefore, animations and simulations are not suitable for capturing students’ intuitive ideas. In contrast, creating simple SMAs became very easy, fast, and accessible for students due to technical innovations. Thus, SMAs can be a good starting point for the analysis and activation of students’ resources on reaction processes.

Second, the type of models used in the SMAs must be reflected. Since the entities (molecules, atoms, reactions. . .) studied in chemistry are not visible, the use of models is inevitable. However, it is well-known that the translation of representations, especially abstract formulas, and signs, is difficult for students and may hinder productive learning [55,56]. The use of spatial three-dimensional models may thus be helpful, especially when the models are self-made [57]. Commercially available molecular construction kits do not allow animating, for example, the course of an S_N2 reaction. Furthermore, students are strongly guided and limited in their ideas due to the restricted number of manipulations in molecular building kits. However, simple plasticine balls can be used as models for atoms. This kind of model allows students to manipulate structures flexibly and relatively unguided. For the reasons discussed, this study will investigate using SMAs with plasticine models to represent reaction mechanisms.

2. Research Objectives

The main goal of this study is to analyze students’ intuitive ideas about reaction processes. Since context is known to be the critical factor for the activation of resources [1], nucleophilic substitution reactions were chosen as a typical organic reaction mechanism. For the analysis, SMAs were used in a dual function: First, students were asked to model their ideas about reaction processes with SMAs. Later, they were asked to reason about two presented literature-based SMAs. These data sources were used to address the following specific research questions:

- (I) How do students intuitively imagine the reaction processes of a nucleophilic substitution reaction?
- (II) What resources do students activate to evaluate different reaction pathways for nucleophilic substitution reactions?

3. Materials and Methods

The empirical methodology is outlined below. First, an overview of the study design is provided. Then, the sample is characterized and the method for qualitative content analysis

is described. The method for the analysis of SMAs is newly developed and is therefore presented in more detail at the end of this chapter.

3.1. Design and Setting of the Study

A qualitative study design seems most appropriate for a detailed analysis of student resources. Data for this study were collected during a visit to an after-school laboratory for high school students. The following is a brief description of the intervention to help situate the study. The out-of-school laboratory “A Look Behind the Reaction Arrow” was designed based on experiments developed in our group [12,58,59] for high school students in grades 11 to 13. The out-of-school laboratory is installed at a large university in the German state of Baden-Württemberg and is visited by school classes together with their teachers during school hours. The visit to the laboratory was led by the two first authors of this study. Students pursuing a Master of Education in Chemistry supervised the high school students during their visit. In Baden-Württemberg, reaction mechanisms were not part of the high school curriculum but will be part of the school curriculum from the school year 2023 [60]. Therefore, the students did not explicitly learn about reaction mechanisms in school before visiting the out-of-school laboratory. The out-of-school laboratory aims to give students a first insight into process-oriented organic chemical reactions. Students investigate reaction mechanisms using scientific methods in four experimental units. For practical reasons, students visit the units in different order. One unit uses colored intermediates to reason about the mechanisms of an electrophilic addition reaction at lycopene [58]. Another unit employs competition experiments with luminous bubble tea to illustrate the mode of function of antioxidants [59]. Computational chemistry was employed to explore energetic aspects of the reaction of chlorine and hydrogen gas. Most important for this study is the unit focusing on nucleophilic substitution reactions [11].

In this study, data were collected at three different times during the visit to an out-of-school laboratory, as shown in Figure 2. Before the experimental work, the high school students were divided into groups of two or three. The students gathered in a seminar room and were asked to complete the sentence “In the course of a reaction . . .” on sticky notes immediately after the welcome and before any content introduction. The purpose of this question was to collect students’ spontaneous ideas without being influenced by any content.

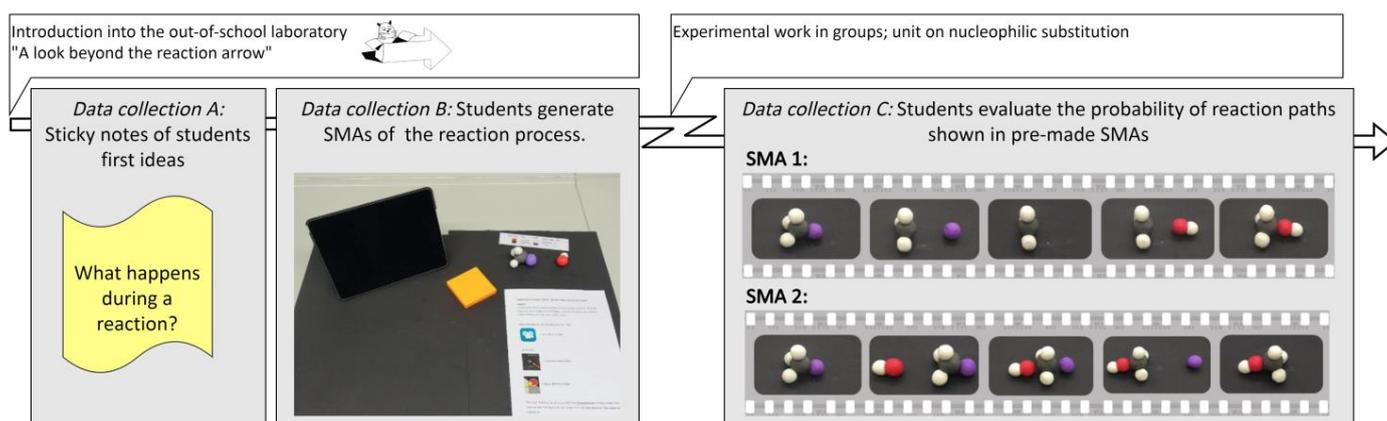


Figure 2. Data collection points during the visit to the out-of-school laboratory “A look beyond the reaction arrow”. A: Example of sticky notes on intuitive ideas of students about “what happens during a reaction”. B: Typical setup for the generation of SMAs by students. C: Evaluation of pre-made textbook style SMAs. The full SMAs can be found in the Supplementary Materials.

A second set of data was collected immediately after providing some details about the out-of-school laboratory. The students were told that they were going to gain further insight into the nucleophilic substitution reaction. They were asked to think about how

they would expect the reaction to occur. Therefore, a tablet with the app “Stop Motion Studio” [61], a short introduction on how to use the app, a simple plasticine ball model of bromomethane and a hydroxide ion, the reaction equation with Lewis structures, and color code legend were provided (see Figure 2, data collection B). The exact wording was: “In your group, create stop-motion videos showing step by step how the reactants react with the products. Feel free to create several videos if you have several ideas.” (Translated; original in the Supplementary Materials [SM].) The benefits of using SMAs for analyzing student ideas on processes are described above. While the creation of such animations used to be very cumbersome just a few years ago, modern apps allow a very intuitive and fast creation of SMAs. The use of the app was no problem for the pupils. In contrast, some of them even used additional app settings that were not mentioned in the brief introduction sheet. Plasticine balls were chosen as a model due to their high versatility. Students had around 15 min to create their SMA(s), and most students finished before time.

Data collection point C was implemented in the unit on nucleophilic substitution reactions. First, students watched two SMAs showing an S_N1 and an S_N2 reaction mechanisms (for screenshots, see Figure 2, data collection C; for complete SMAs, see Supplementary Materials). These SMAs were prepared in advance by the authors of this study based on textbook mechanisms [62] and used the same reaction, model, and technology as the students used at the beginning of their laboratory visit. The following work assignment was given: “On the iPads you will find two video examples for the course of a reaction, just as you created one earlier. Watch the videos and name the central difference between the two reaction courses. Discuss how the reaction is most likely to take place from your point of view. Please answer in as much detail as possible (minimum of five sentences)”. (Translated; original in the Supplementary Materials.) After ten minutes, the answers of the students were collected. Then, the students performed nucleophilic substitution reactions with a primary and a tertiary bromoalkane. Precipitation reactions of bromide were used to allow conclusions on the kinetics of the different reactions. Further details and experimental procedures are described in the literature [12].

At the end of the visit, a short survey was handed out. It asked for age, class, gender, and performance in chemistry. Scientific interest and self-concept of ability in chemistry were measured with scales using slightly adapted items from the literature [63–66]. For the scales, very good Cronbach’s alpha values of $\alpha = 0.88$ – 0.89 were obtained. The collected data are used to describe the sample in Section 3.2. Dependencies of the measured characteristics were checked against the results of this study. As no difference became significant, these analyses are omitted in the manuscript. Teachers filled in another survey to rate the out-of-school laboratory. This survey asked if reaction mechanisms were already explicitly taught in the school classes visiting the out-of-school laboratory. All teachers answered no to this question.

Participation in the study was voluntary and not mandatory for the visit to the out-of-school laboratory. Informed consent was obtained from all participants. Students that did not want to participate followed the same procedure in the out-of-school laboratory as the others, but their data and videos were not collected or saved. The study is part of a larger research project on student understanding of energetic aspects in chemical reactions. The research project was approved by the Faculty of Economics and Social Sciences Ethics Committee of the University of Tuebingen.

3.2. Sample

Fifty-five German high school students from five different courses participated in the study. All students chose chemistry as a main subject (“*Leistungskurs*”) and visited the class 11 to 13 of a German high school (“*Gymnasium*”). The mean age was 17.7; 55.4% of the students identified as female and 41.1% as male. Scientific interest was broadly distributed with a mean of 1.6 and a standard deviation of 1.1 on a Likert scale from 0 (very high interest) to 4 (very low interest). The self-concept of ability in chemistry had a mean of 1.5

with a standard deviation of 0.9 on a similar scale. The high standard deviations for both scales illustrate the diversity of the sample. All data were collected in the Summer of 2022.

The students were divided into 23 groups of two to three students for the whole day. All groups were assigned a pseudonym to link the data collected for the different tasks. The groups created a total of 60 sticky notes, 32 SMAs, and 53 written explanations.

3.3. Analysis of Student Statements

All hand-written statements and sticky notes of students were transcribed one-to-one to a digital format. Neither grammatical nor orthographic mistakes were corrected. All analyses were performed with the help of MaxQDA [67].

The keywords noted by students on the sticky notes were categorized by a structured content analysis, as described by Kuckartz [68]. Categories were formulated deductively and loosely based on chemical core ideas clustered around the main topics “chemical reaction” (e.g., donator–acceptor-relationship, reversibility, chemical equilibrium), energy (e.g., energy conversion, kinetics), and structure and properties of substances and their particles (e.g., chemical bonding, functional groups) [69].

Student reasoning on the probability of the two reaction paths as shown in the pre-made SMAs was also analyzed by a qualitative content analysis [68]. The first step was to analyze which of the two reaction paths shown in the videos seemed most likely to the students. As only three answers (video 1, video 2, both) could be expected, the categories were formed accordingly. Then, the complete text was analyzed for the knowledge resources that students employed. The categories for these knowledge resources were formed inductively; the smallest interpretation unit was a half sentence.

Thirty percent of the data material was re-coded by an independent research assistant. For the intercoder reliability, a value of Cohen’s kappa of $\kappa = 0.72$ was found, which is an indicator of good agreement.

3.4. Analysis of Student-Generated SMAs

While the qualitative content analysis of written answers is well-established, the analysis method for the SMAs had to be newly developed. First, a purely qualitative analysis of the SMAs was tried through the generation of focused summaries of the SMAs. A systematic evaluation failed due to the abundance of descriptions. Hence, a quasi-quantitative analysis of the SMAs seemed to be a more sophisticated way to derive meaningful categories. Therefore, video data were translated into other representations that can be analyzed more easily, e.g., mathematical descriptions of the occurring chemical structures. First, the SMAs were separated into single image files (Figure 3a). The processes described with SMAs are mainly reflected in the change between two single images. Consequently, student ideas or concepts are also better presented through the changes between pictures than in a single picture itself. Thus, the elementary movements of the single plasticine balls from one to another picture were analyzed. A two-dimensional grid was laid over each picture of one SMA, using software called “digitizeit” [70]. The coordinates for each plasticine ball were determined. From these coordinates, the distance of all plasticine balls to each other can be calculated and normed against the start distance. In 25 of the 32 SMAs, only the distance of the red and purple balls to the black ball varied. For dimension reduction, only these distances were further analyzed. The seven SMAs with other varying distances were analyzed separately (see section “Results” for details). The described method yielded distance diagrams, as depicted in Figure 3c. Due to viewing perspectives, some distance changes were artefactual or not properly seen in the diagrams. For example, the movement of one plasticine ball behind another one resulted in a two-dimensional distance near 0. Hence, the diagrams were carefully corrected by comparison with the original SMAs. For eight SMAs, these corrections were performed independently by two different researchers yielding an excellent intercoder reliability indicated by a Cohen’s kappa of $\kappa = 0.83$. The different movements identified by this quantitative analysis yielded the category system for the SMAs presented in Figure 4. SMAs within the categories were further compared,

and additional features were further analyzed qualitatively (e.g., the movement of atoms in frames 4–6 of Figure 3a).

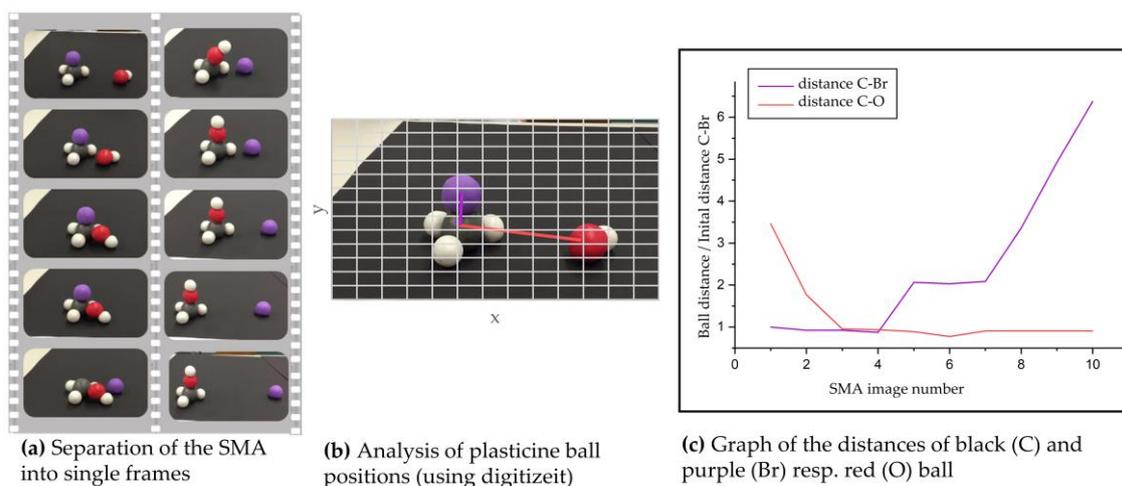


Figure 3. Steps of SMA analysis (from left to right): (a) Separation of the SMA into single frames; (b) Analysis of the geometrical position (x , y) of the plasticine balls in each frame with the help of a grid (symbol picture, originally performed with “digitizeit” [70]); (c) Diagram of relevant distances in the SMA.

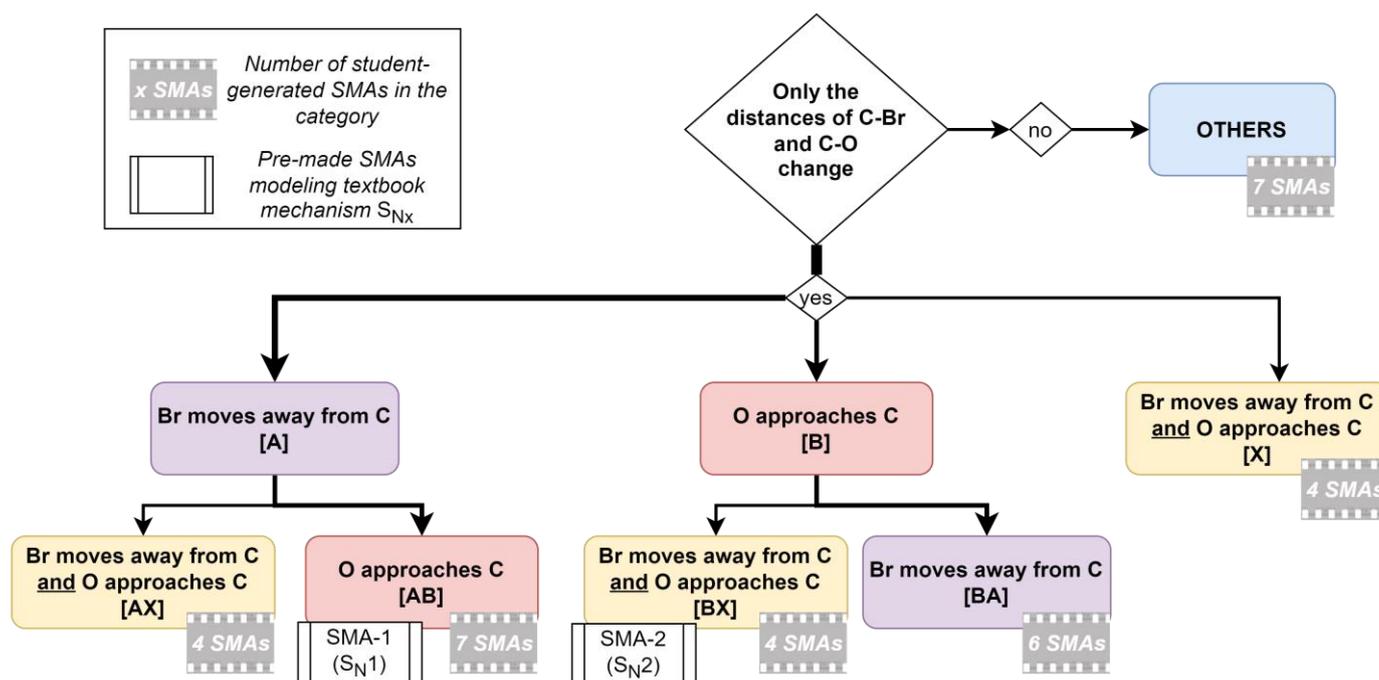


Figure 4. Category system derived from the qualitative analysis of student-generated SMAs. The digit in the grey box indicates the number of student-generated SMAs in the relevant category. SMA-1 and SMA-2 are the pre-made SMAs, as shown in Figure 2, that were categorized similarly to the student-generated SMAs. Screenshots of anchoring examples for the central categories are provided below.

4. Results

The research questions structure the presentation of findings. Findings from one phase may be used in different sections of the Results section and do not necessarily reflect the order of the phases during data collection.

4.1. How Do Students Intuitively Imagine the Reaction Processes of a Nucleophilic Substitution Reaction?

4.1.1. Typology of Student-Generated SMAs

For ease of description and understanding, the black plasticine ball will be referred to as “C”, the red plasticine ball as “O”, the purple plasticine ball as “Br”, and the white plasticine ball as “H”. Accordingly, C-Br describes the distance between the black and the purple balls and C-O the distance between the black and red balls. This nomenclature corresponds to the legend given to the students for creating the SMAs. However, this nomenclature is not intended to imply that all students interpreted the sphere model correctly when creating the SMAs. The purpose of the nomenclature is to simplify the description and understanding of this chapter.

A total of 32 SMAs were generated by the 22 groups in this analysis. The mean number of frames was 8.7. Categories were derived from the distance plots as described above. The main movements of the clay balls were analyzed. In seven of the SMAs, a distance other than C-Br or C-O became relevant. These SMAs were placed in the OTHER category. In all other SMAs, only three main movements were observed:

- A: Br moves away from C (included variant: Br and O move away from C)
- B: O approaches C (included variant: O and Br approach C)
- X: Br moves away from C and O approaches C.

Some closely related variants have been included in the main categories. A closer analysis of the relevant SMAs suggests that these variants are not intended to represent a different idea or concept but rather were created for practical reasons to simplify the presentation. Each time a different one of these three fundamental movements was shown in the SMAs, a new subsection was defined in the analysis. For most SMAs, two subsections were sufficient to describe different movements. Only four SMAs had three to five different subsections defined. However, the changes described in these latter subsections seem to be of less interest to this study. For example, they show the movement of Br after O has fully approached C (i.e., a new bond has been formed). Therefore, only the first two subsections were considered for the formation of the categories shown in Figure 4.

Category AX and AB: In eleven of the students’ SMAs, Br first moves away from C before C-O decreases eventually. In four of these animations, O begins to approach C, while Br is still moving (category AX). In the other seven SMAs, all processes were shown one after the other, as shown in Figure 5. Also, SMA-1 (modeling a textbook S_N1 reaction mechanism; see Figure 2) is best described by this category. However, the pre-made SMA differs in one central point from all the student-generated SMAs in this category: In an S_N1 reaction, a carbocation is formed. Thus, the geometry of the molecule changes from tetrahedral to trigonal planar. Accordingly, in SMA-1 the position of all three Hs changes during the abstraction of Br. However, none of the student-generated SMAs—except those in the “OTHER” category that depict bond cleavage—shows any movement of the Hs.



Figure 5. Example of an SMA of Type AB. The student-generated SMA was separated into single frames, cropped, and shortened (10 out of 14 frames). Full examples of SMAs for all categories can be found in the Supplementary Materials.

Category BX and BA: In 10 of the SMAs, O first approaches C. In four of these SMAs, Br begins to move away while O is still approaching (category BX). This category also best describes SMA-2, which models a textbook S_N2 mechanism. In six student-generated SMAs, Br only begins to move away after O stops its approach (BA; see Figure 6). The simultaneous movement of Br and O is thus completely avoided. Again, all animations in this category differ from SMA-2 in one central point: In S_N2 mechanisms, the nucleophile attacks from the backside due to steric reasons. Consequently, in SMA-2 O approaches from the backside. In contrast, in all student-generated SMAs, O approaches from the same side of the black ball that Br is bound to. As a consequence, this side of the black ball became “overcrowded”. Hence, students had to rearrange the position of the red ball on the black ball after the purple ball had been distanced. Such an archetypical arrangement can be seen in Figure 6.

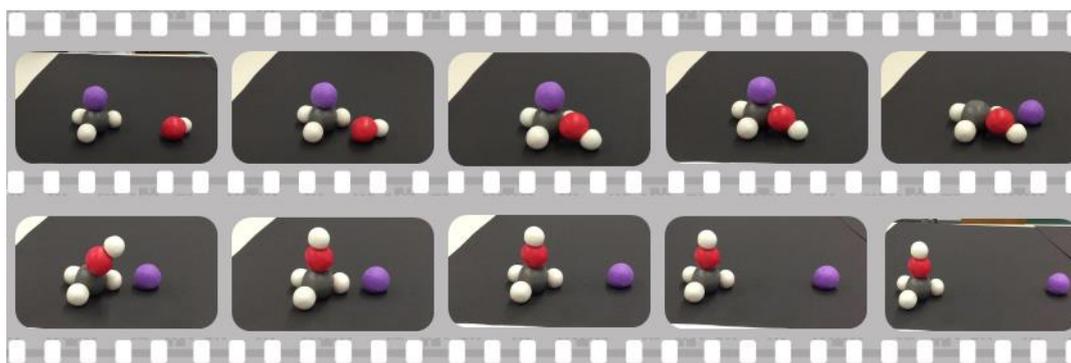


Figure 6. Example of an SMA of Type BA. The student-generated SMA was separated into single frames and cropped. Full examples of SMAs for all categories can be found in the Supplementary Materials.

Category X: Four SMAs show simultaneous movements of O and Br in between all frames except for two SMAs, in which Br stops moving in the last few frames. All SMAs in this category are rather short, with only three to eight frames. Due to this small database, the interpretation of this SMA type is difficult. Especially for SMAs with only three pictures, it cannot be distinguished if students wanted to point out the simultaneous movement or if they just tried to find the shortest possible answer. Caution was undertaken to not overinterpret these results.

Category OTHER: In seven of the 32 SMAs, other distances than Br to C and O to C changed. They were classified in the category OTHER. In five of these SMAs, intermediates (other than carbocations) were formed. Chemically, these intermediates could be interpreted as models for H_2O (as in the example of Figure 7), HBr, or HOBr. The two other SMAs did not include actual intermediates but attributed an active role in the reaction process to at least one H.

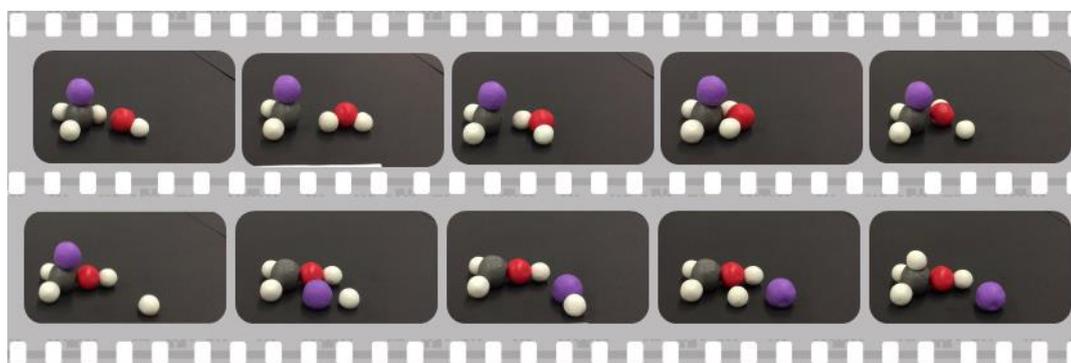


Figure 7. Example of an SMA of Type OTHER. The student-generated SMA was separated into single frames, cropped, and shortened (10 out of 14 frames). Full examples of SMAs for all categories can be found in the Supplementary Materials.

4.1.2. Consideration of Different Reaction Paths in Student-Generated SMAs

Students could create several SMAs. This was triggered by the sentence: “*Feel free to create several videos if you have several ideas*”. The wording was chosen to have minimal impact on the students’ initial ideas while allowing them to provide different response paths. Thirteen of the groups provided only one SMA, eight groups provided two SMAs, and one group provided three SMAs.

From these eight groups, two groups produced SMAs that were categorized equally in Figure 4. Thus, the differences between the SMAs were minor and, to the extent accessible by the used methods, did not reflect different ideas about reaction mechanisms. The alternative SMAs of five groups were categorized as OTHER. This means that a very different reaction mechanism, including the formation of an intermediate, was demonstrated. Conversely, all but one group that produced an SMA in the OTHER category also produced a second SMA from one of the main categories.

Only two groups produced two SMAs that fell into two different main categories, i.e., none of their SMAs involved other intermediates. However, the two SMAs of one group consisted of only three frames, making it difficult to infer the underlying ideas. The two SMAs of the other group were categorized as AB and AX. They differ only in an additional rotation of the hydroxy group.

Thus, no single group showed a stepwise and concerted mechanism in two different SMAs.

4.1.3. Students’ Assessment of Pre-Made SMAs

Finally, in Data Collection C, students viewed SMA-1 and SMA-2, which represented the textbook mechanisms. Students were then asked individually which mechanism seemed more likely to them. There were no differences in preferences within groups; all students argued for the same SMA. In total, 15 groups argued that SMA-2 (S_N2 mechanism) was more likely. Only four groups argued for SMA-1. All groups showed a clear preference, and no group discussed whether both mechanisms could be possible. The students’ reasoning is discussed below. Of the student groups that generated SMAs starting with the approach of O and C (categories BA and BX), 90% also chose SMA-2 as the more likely reaction process. Surprisingly, the majority (67%) of the students who generated an SMA starting with the abstraction of Br (categories AX and AB), i.e., animations similar to an S_N1 mechanism, also chose SMA-2 as the more likely mechanism.

4.1.4. Summary

All high school students were able to model some reaction processes of a nucleophilic substitution reaction by generating SMAs. About the same number of SMAs resembled S_N1 mechanisms as S_N2 mechanisms. However, no group proposed S_N1 -like and S_N2 -like mechanisms as two different reaction pathways. In contrast, rather unusual reaction pathways were proposed as an alternative. After being shown SMAs of the textbook mechanisms, most students rated the S_N2 -like mechanism as more likely—including most students who had previously modeled an S_N1 -like mechanism. Simultaneous movement of atoms, backside attacks, and movement of hydrogen atoms were shown rather rarely.

4.2. What Mental Resources Do Students Activate to Evaluate Different Reaction Pathways for Nucleophilic Substitution Reactions?

Up to this point, the student-generated SMAs and their evaluation of the ready-made SMAs have been discussed from a descriptive perspective. In order to gain insight into students’ underlying mental resources, students’ written explanations were examined. First, the sticky notes from data collection point A were analyzed to collect students’ initial associations with reaction processes.

4.2.1. Students' First Ideas on Reaction Processes

Sixty sticky notes completing the sentence “*In the course of a reaction. . .*” were collected. If different ideas were noted on one sticky note, they are counted twice below.

- Twenty-five of the answers focused on the formation of new products in chemical reactions on a macroscopic scale, e.g., “. . . *new compounds with new properties are built*”.
- Ten answers referred to products in chemical reactions but on a sub-microscopic scale: “. . . *atoms meet*”.
- Six answers referred to other reaction-related concepts like chemical equilibrium or the donator–acceptor-principle.
- Twenty-two answers involve energies, almost all of them on a macroscopic scale: “. . . *energy is released, or energy is added*”.
- Only four answers comprised bond-breaking or bond-making or a structural change of the atoms.

Hence, for most of the students, chemical reactions seem to be most dominantly connected with macroscopic processes [71].

4.2.2. Ideas Activated to Argue on the Probability of Reaction Paths

In data collection point C, students were asked to evaluate which of the textbook-based animations SMA-1 or SMA-2 (see Figure 2) are more likely to happen. These explanations are the richest data source for insights into students' thinking. In their explanations, almost all students used chemical names, such as carbon atom, hydrogen, hydroxy group, or more general chemical concepts, such as product or particle, to describe the plasticine balls. Only five out of 321 descriptions argued on the model level talking about *purple balls*. A few groups conflated the shown atoms, e.g., talking about “ NH_3 ”. Nevertheless, the vast majority correctly assigned the model. Therefore, it seems reasonable to assume that the groups, in general, were able to interpret the plasticine model. All students in the sample were asked to give an individual answer to the question. However, since the students worked together in groups of two or three throughout the day, the answers within a group were often very similar. Therefore, the following section refers primarily to group responses. When differences within groups are discussed, they are mentioned explicitly. The full category system with anchoring examples can be found in the Supplementary Materials.

Students used a rich variety of mental resources on chemistry to argue about the reaction processes modeled by the SMAs. They were grouped into the **categories in bold**. Most frequently, students argued using **chemical bonds**. Over 60% of all student groups (14 groups) mentioned chemical bonds in any context. However, the arguments within this category were quite different. Six groups discussed some kind of “**bonding sites**” at the central atom. They used very different wording to describe that idea, including “*place*”, “*spot*”, “*gap*”, or “*taking over a bond*”. One student argued that SMA-1 is more likely, because “*in video 2 no bond was free until the bromine was gone, but the [hydroxy] group was already binding to the molecule. In video 1, the first bond to be released is the one that is then filled with the group*”. Another group preferred SMA-2, as it shows that “*bromine is repelled because it no longer has a place due to the connection of the OH group*”. Closely related to this argumentation pattern, four groups focus on the **number of chemical bonds**, because “*temporarily there are five bonds*”. This argument was also used both for and against S_N2 mechanisms. Some groups argued that SMA-2 seems more likely “*because the addition of the hydroxyl group causes the C atom to form too many bonds and therefore the Br must be split off (\rightarrow octet rule)*”. In contrast, other groups argued that SMA-2 is unlikely, “*since carbon is less likely to form 5 bonds*”. Three groups argued for a **competition of different bonding partners**, as “*the OH^- ion and the Br^- compete for the bond with the carbon atom*”. Only two students argued with the **position of the H-atoms** at all, e.g., “ *OH^- approaches HC_3-Br [sic!] and forces the two hydrogen atoms to the outside*”. Interestingly, in both cases, fellow students in the relevant groups omitted this aspect in their argumentations.

Twelve of the groups judged the probability of the two SMAs by their **plausibility**. The main argument in that regard was that it is not “realistic” that bromine would leave “just like that”, “for no valid reason” or “without external influence”. In contrast, in SMA-2, “the hydroxide ion is the reason that the bromine splits off and not as in [SMA-]1 simply like this”.

Interactions between the different particles were mentioned by 11 groups. The students named several interactions that could play a role in the mechanism, e.g.:

- “OH⁻ is strongly negative and thus repels the bromine atom [sic!]”
- “the positive partial charge of the C atom attracts the partial negative charge of the OH⁻ particle”
- “the positive pole of H₃CBr first approaches the negative pole of OH⁻”.

While these arguments refer to electromagnetic interactions, several students did not specify the nature of the interactions in more detail and only referred to attraction or repulsion in general; one student compared these forces to “a magnet”. The other four groups referred to the **proximity or distance** of particles. From that perspective, “the OH⁻ molecule [sic!] confuses the structure of the CH₃-Br molecule by approaching it”.

The **electron configuration** of the relevant species was mentioned by four groups. They argued, for example, that in SMA-2 “OH⁻ gives the molecule an extra electron. Since it now has one too many, it can repel the bromine”. Another group argued in favor of SMA-1 that the “free electron pair to which OH⁻ can bind is present only when bromine detaches”. It should be highlighted that students discussed these questions even though electrons, bonds, or free electron pairs were not represented at all in the SMAs.

Only sporadically, students related to some kind of “intermediate state” (two students) or “energetically reasonable” reaction steps.

4.2.3. Students’ Wording to Describe Bond-Breaking and Bond-Making

In analyzing students’ arguments, the variety of words students used to describe the processes of bond-breaking and bond-making was striking. This wording can provide insight into students’ thoughts about these processes. Therefore, the students’ wording was analyzed and presented as a word cloud in Figure 8. All verbs describing bond-making were used in active voice only. For bond-breaking, verbs in active and passive voice were employed. For both concepts, the ideas of proximity and “attachment” dominate.

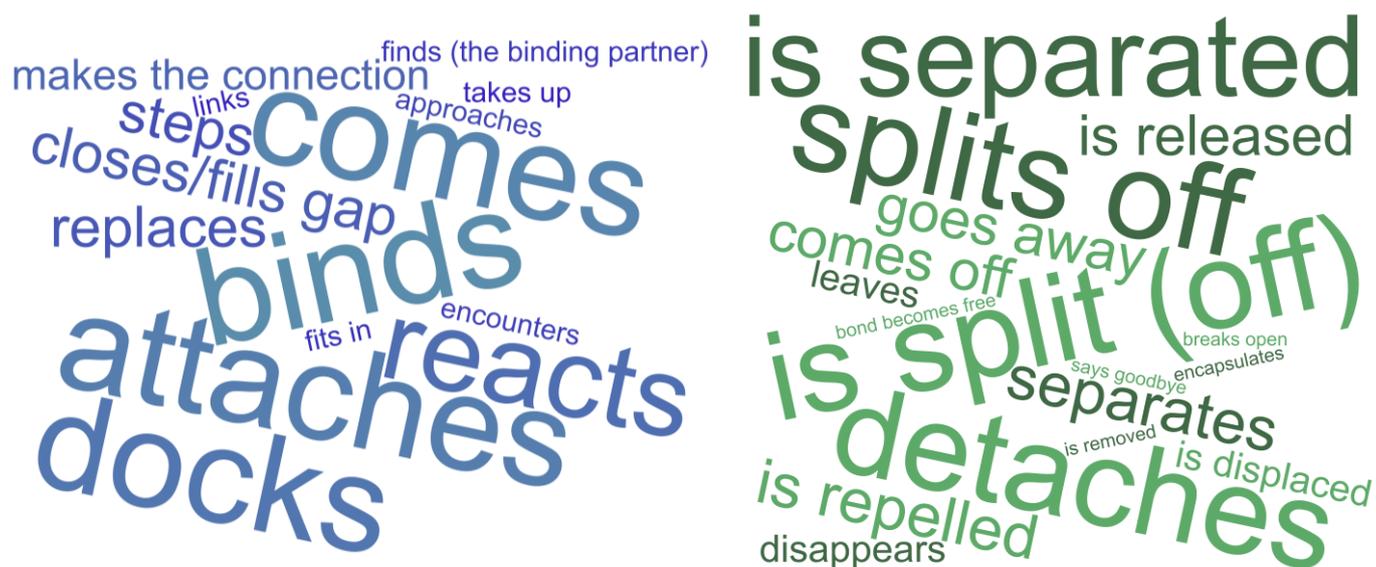


Figure 8. Word clouds of students’ wording describing bond-making (left) and bond-breaking (right). Font sizes display the frequency of the wording used; full details can be found in the Supplementary Materials.

4.2.4. Summary

High school students used arguments on **chemical bonds**, including the **number of bonds**, **“bonding sites”**, and **competition of bonding partners**, on **interactions**, **electron configuration**, and **plausibility** to reason about different reaction paths. The argument on plausibility was only used to argue against S_N1 mechanisms but never against S_N2 mechanisms. In contrast, some other concepts like interactions, number of electrons, or arguments on “bonding sites” were used by students arguing in favor of both reaction mechanisms.

5. Limitations

Students’ ideas are influenced by chemistry courses and teachers. Therefore, it is not possible to distinguish students’ intuitive ideas from those influenced by previous learning. This limitation emphasizes the need to assess students’ learning conditions in situ in the classroom. SMAs can be a reasonable method to realize this analysis.

Both the prefabricated SMAs and the clay model itself have several limitations. The influence of the solvent is neglected in the modeled reaction mechanisms. This may be of particular importance, as an S_N1 reaction can only be properly understood if the stabilizing role of solvent–solute interactions is considered. Furthermore, the different sizes of atoms are not adequately considered in the clay model. This may affect students’ reasoning. Presumably, a “bigger purple ball”, as shown in Figure 9, would have helped students to argue with a backside attack. It is also not possible to distinguish if the physical model or other influences (e.g., pre-knowledge, or the prompt itself) helped students to include bonds and electrons in their explanations.

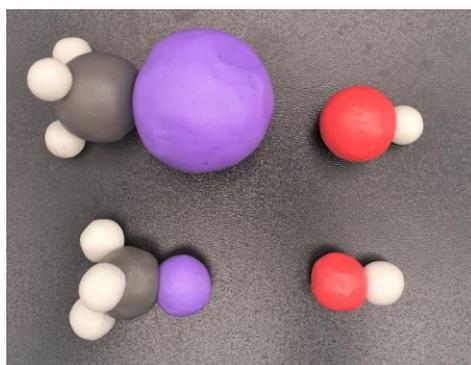


Figure 9. Comparison of the used plasticine model (bottom) and the revised plasticine model with realistic proportions based on atomic radii [72,73].

Orrayd [48] emphasized that many students’ ideas are best captured in the process of modeling itself. For practical reasons, it was not possible to observe or videograph the creation of the SMAs. This analysis could provide even deeper insights into students’ conceptions. Also, in school settings, it may not be possible to observe the modeling process for all students in a class. This study proves that student conceptions can still be properly analyzed.

6. Discussion and Implications

Most student groups in the sample were able to generate SMAs that described some kind of reaction process. Before focusing on shortcomings or scientific misconceptions, it is important to emphasize that almost all students in the sample were able to model the process of an unknown reaction at the molecular level. In doing so, they activated a wide variety of resources. Only a few groups produced three-frame SMAs, which do not allow deeper insights into the reaction processes, and referred only to descriptive arguments of the other SMAs. In contrast, the vast majority of groups built their explanations on ideas that were not explicitly represented by the clay model used, such as bonds or electron configurations. Thus, these resources are a rich foundation for the construction of new

knowledge. Nevertheless, the differences between students' and experts' thinking about reaction mechanisms should not be surprising. Some of the key points will be discussed in more detail.

In general, students do not use ideas coherently. Throughout the results reported above, high school students do not refer to a coherent concept for judging reaction mechanisms. Instead, many of them used everyday logic to puzzle the product. Similar reasoning can also be observed when university students develop reaction mechanisms [24]. One of the most striking observations was that a large proportion of the students who created an S_N1 -like SMA tended towards an S_N2 -like SMA when evaluating the pre-built SMAs. This may be due to the fact that these students initially had no idea of a concerted mechanism, or that the presentation of the prefabricated SMAs activated additional cognitive resources. Interestingly, the significantly higher agreement with the S_N2 mechanism is in line with the historical development, where carbocations were seen as rare exceptions [7]. Furthermore, high school students initially seem to understand chemical reactions primarily at the macroscopic level, as evidenced by their definitions of reaction processes. However, most groups were able to activate various resources at the molecular level when triggered. The use of the plasticine model and SMAs can help to shift the focus to the submicroscopic level, even without in-depth knowledge of chemical formalism.

A focus on sequence and concertedness of reaction steps is not intuitive. Within all student-generated SMAs, the two basic reaction mechanisms for nucleophilic substitution reactions— S_N2 and S_N1 —were almost equally distributed. Thus, both reaction pathways seem to have a certain logic for high school students. However, no group showed both of these different reaction pathways in their SMAs. Therefore, it seems that students are less aware of issues of order and concertedness of reaction processes. In order to model different reaction paths, students almost always used intermediates. The SMAs in the OTHER category were almost exclusively provided as a secondary reaction pathway. It seems that students thinking about alternative reaction pathways first of all think about other intermediates, i.e., from a thermodynamic perspective. Kinetic aspects, like “how” the intermediate or product are formed, do not seem to be intuitively considered as “other” pathways.

Students' suggestions of unusual reaction pathways are good learning opportunities. To an experienced chemist, some of the intermediates and pathways in the OTHER category may seem illogical or unreasonable. It may be helpful for chemistry teachers and instructors to be aware that all of these reaction paths are conceivable and lead from the reactant to the product. Only through their experience with other reaction mechanisms can experts judge the likelihood of these pathways [6]. Indeed, the history of science has shown that the most straightforward mechanism is not always the energetically most favorable. For example, for aromatic nitration, most chemists propose and still teach a reaction mechanism via a direct polar attack of a nitronium ion. However, quantum chemical calculations show that a rather contra-intuitive single electron transfer is most likely part of the mechanisms [74,75]. Thus, in general, all hypotheses about reaction pathways must be tested experimentally, whether in the laboratory or by quantum chemical calculations. Therefore, the ideas of high school students presented in the SMAs should be evaluated as possible solutions to a chemical problem. Some of the proposed mechanisms can be directly attributed as unlikely based on general principles derived from other mechanisms: For example, one can argue that the mechanism proposed in Figure 7 is unlikely because it is known from many calculations that single protons (or H-atoms) are energetically very unfavorable.

Concerted reactions seem to be rather unintuitive. In general, stepwise processes were shown very often, while concerted steps (movement X) were rather rare. Even in S_N2 -like SMAs, concerted movements of Br and O were often omitted (type BA). Only a few groups showed simultaneous movements (type BX), which are typical for concerted mechanisms. It could be for similar reasons that all the students neglected the movement of the hydrogen atoms in all the videos (except the H abstraction in the category OTHER). Students did not consider that the position of the hydrogen atom on the central carbon

could change during either the formation of carbocations or the attack of the hydrogen group. Obviously, it is easier to focus on one movement than on a multitude of changes. However, atomic motion does not occur in isolation in almost all chemical processes. Therefore, students can gain a new perspective on chemical reactions by learning about concerted reaction mechanisms.

Binding is often understood to occur at fixed places. For S_N2 -like SMAs (both in category AB and AX), backside attacks were never shown by students. Even in S_N1 -like SMAs, the hydroxy group was bonded at the same position where the bromine was previously bound. It seems that many students somehow expect bonding to “happen” only at specific places on an atomic surface. In fact, students often used phrases such as “no bond was free”. This type of thinking may be reinforced by the use of molecular modeling sets that have well-defined junctions. While these types of models are certainly very useful for modeling organic chemical reactions, one should also be aware of their shortcomings. The use of a variety of models, such as plasticine models, can help to reduce such alternative conceptions. In addition, the language used by students to describe bond-making and -breaking indicates the diversity of students’ understanding of chemical bonding. This is consistent with empirical research suggesting that students’ understanding of chemical bonding is rather poor [41,42,76].

Awareness of the duality of mechanisms and border mechanisms must be learned. Until the 1930s, the concept of singularity reaction mechanisms was widely believed [7]. Similar reactions should always occur in similar ways. Therefore, Ingold’s proposal of two reaction mechanisms seemed a strange idea to many chemists. Interestingly, also in this study, no student considered the possibility of concurrent reaction mechanisms but all students unambiguously argued for one of the proposed pathways. There was also no evidence that any student understood the mechanisms shown as borderline cases with the actual mechanisms being in between. Grove and Bretz [77] used Perry’s scheme to analyze students’ epistemological development. In agreement with our findings, they reported that many students adhere to dualistic “black and white” thinking. The parallels with the history of science show that the idea of multiple reaction mechanisms is not a simple or intuitive one.

Therefore, it is not our intention to highlight students’ deficits by describing the differences between students’ intuitive ideas about reaction processes and scientific knowledge. On the contrary, all of the above points outline the potential of students’ ideas. Discussing students’ proposals appreciatively and seriously is not only useful from a pedagogical point of view. It is also a way of demonstrating to students on the spot how scientific inquiry works, and of training them in the skills of scientific reasoning. This can help students reflect on their epistemology and understanding of natural processes.

Students’ arguments against textbook mechanisms provide a good starting point for further learning. The high school students in the sample provided various arguments for and against reaction mechanisms. Central arguments were found against both textbook mechanisms. In the case of the S_N1 mechanism, many students criticized that there is no plausible reason for the bromine to leave the molecule. First, students are right: Solvent molecules were not represented in the model. For the thermodynamic stability of the carboxylate, the stabilizing interaction between the solvent molecules and the carboxylate plays a crucial role. This limitation of the model used here (and of most other commonly used models) should be explicitly discussed. On the other hand, the result can also be understood from the perspective of ‘common sense chemistry’. Talanquer [78] argues that inexperienced chemists expect a clear causal agent to explain processes. The example of stepwise mechanisms can thus be a good learning opportunity on the arbitrary and reversible nature of many submicroscopic processes.

Nor is the central argument against S_N2 meaningless, since five bonds on a carbon atom violate the octet rule. In fact, students use the octet rule as a central resource in many contexts [41,42]; and the octet rule is often understood as a concept rather than a mnemonic [79]. Learning about transition states in the context of S_N2 mechanisms can thus

be an opportunity for students to reflect on the meaning of the octet rule. They can learn that almost always a less stable state (i.e., the transition state) must be crossed to reach another energetic minimum.

In general, it seems that students tend to intuitively use arguments based on plausible causes and consequences. Students' reasoning about these ideas may be sharpened by learning about reaction mechanisms. Therefore, it is important to avoid making reaction mechanisms seem arbitrary. Omitting "details" such as solvent or substituent effects may disrupt the causal structure of arguments. How to teach reaction mechanisms coherently and appropriately, especially at the high school level, should be further investigated.

7. Conclusions and Suggestions for Future Research

This study investigated high school students' intuitive resources about reaction mechanisms. The results suggest that students can model reactions at the particle level using a variety of cognitive resources from different domains. Students also activated resources for their explanations that are not represented in the model itself. However, certain aspects of reaction mechanisms, such as questions about concertedness, the duality of mechanisms, or the probability of certain intermediates, are not intuitive.

Thus, teaching reaction mechanisms in high school can help students make new mental connections and revise their mental schemas. In practice, students' intuitive ideas provide a meaningful starting point for learning about mechanisms.

SMA play a central role in this study. Students generated their own SMAs to model the reaction. The different textbook mechanisms were illustrated by pre-built SMAs. This low-threshold technology can be easily implemented in the classroom. Combined with appropriate models, SMAs are a helpful tool to visualize motion at the submicroscopic level. Thus, SMAs can help teachers to easily analyze the resources activated by students "on the fly". In addition, the generation of SMAs activates students' resources, which can support the formation of a productive mental network for reaction processes. In the classroom, this can enable a variety of learning opportunities starting from students' ideas.

In this study, we did not investigate what kind of knowledge helps students to construct reasonable explanations for the reaction processes. However, the results may suggest that a sound understanding of the formation and breaking of bonds is of fundamental importance. It would be of great interest for future research to investigate how different levels of knowledge in different domains (e.g., orbital theory, understanding of energy, concept of chemical reactions) affect intuitive ideas and mechanistic learning. In general, there is a need for much more research on high school chemistry education to provide a solid basis for evidence-based improvements in the promotion of conceptual chemical knowledge from the very beginning of chemistry learning.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/educsci13070759/s1>, 1. Original German wording of work assignment; Figures S1 and S2: Frames of the textbook style SMAs used in Data Collection C; Figures S3–S8: Anchoring SMAs for the different categories; Table S1: Wording of students used to describe bond-breaking and bond-making; Table S2: Category system of students' argumentation in Data Collection C with anchoring examples (in German and English).

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