Good practice report

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Designing a scaffold for mechanistic reasoning in organic chemistry

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Abstract: Designing problems and learning activities is a key factor to initiating students' engagement with the course material and influencing their reasoning processes. Although tasks and problems are a central part of teaching and assessments in the chemistry classroom, they may not engage students in deep reasoning or in a way that is intended through a task. Some problems may cause an algorithmic or a surface approach. Even with designing clever problems, students may not use a larger variety of chemistry ideas and connect them in meaningful ways. Here the idea of scaffolding students' answering process comes into play. Structuring students' reasoning process through instructional prompts or structured worksheets supports students in activating and connecting knowledge pieces in a more meaningful way and positively slows down their fast decision-making process. This paper will discuss the importance of asking questions in chemistry teaching and highlights the idea of contrasting cases, drawn from cognitive psychology, as a task design principle. In addition to having contrasting cases as a good problem format, the idea of scaffolding students' reasoning while solving contrasting cases through the use of instructional prompts that scaffold the reasoning process will be exemplarily showcased for mechanistic reasoning in organic chemistry.

Keywords: contrasting cases; organic chemistry; scaffolding reasoning.

Introduction

Presenting students with a variety of chemical reactions, as it is common in traditional chemistry courses at the tertiary level, often does not engage them to reflect on underlying implicit causes for a chemical phenomenon. Students in general tend to focus on surface features and encode cases in a situation-specific manner (Gentner, 1989). As a result, they have difficulties in retrieving the relevant concepts underlying various cases and often rely on recall (Chi, Feltovich, & Glaser, 1981; Gentner, Loewenstein, & Thompson, 2003). This surface approach is reinforced when cases, e.g. chemical reactions, are examined sequentially, which is typical in traditional organic chemistry courses. One chemical reaction mechanism is presented after another, often without showcasing the similarities and differences. A problem format that has been used widely in educational studies of the last decades is to introduce variation, which means to combine two cases that slightly differ and prompt learners to critique or reflect about the contrasted cases (Bussey, Orgill, & Crippen, 2013). A meta-analysis on studies using the idea of contrasting cases instead of single cases in various disciplines has shown that purposefully designed comparisons help students discriminate more of the possible variables, which are relevant in a problem situation (Alfieri, Nokes-Malach, & Schunn, 2013). Students, who work with contrasting cases are more engaged in discerning critical, differentiating, or common features of two or more cases. The

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extensive research on the use of contrasting cases in various disciplines has revealed two fundamental advantages: First, students notice information they might otherwise overlook, this could be procedural learning, i.e. how to solve a given problem (Rittle-Johnson & Star, 2007, 2009) or conceptual learning, i.e. the deep structure of concepts (Gick & Paterson, 1992; Schwartz & Martin, 2004). Depending on the stage of expertise of the students, different contrasting cases can be grouped together to stepwise develop, apply, or expand a concept (Graulich & Schween, 2018; Schmitt & Schween, 2018).

The idea of contrasting representations can be used as a general instructional tool in various instances. Figure 1 shows exemplary contrasting cases for different contexts. Contrasting case A allows determining students' understanding of the particulate nature of matter, by giving the learner three contrasting drawings. With the three different representations of the particulate level, students are encouraged to discuss different features and thus reflect on their own conceptions. For example, the different colors used for representing the water molecules can provoke discussion about whether molecules of water have the same color as water itself and what meaning color has in representations of the particulate level. The contrasting case can also provoke discussion about the nature of the space between molecules.

Contrasting case B asks the learner to compare common representations of a water molecule. Contrasting cases C and D focus on chemical processes and prompt the learner to explain the differences in activation energy of a reaction step (C) and to reflect on structure-property relationships (D). To solve these cases, students need to consider the electronic structure of the given molecules. In contrasting case C, the phenyl rings around the carbocation stabilize the positive charge due to resonance effects, whereas the methyl groups can only stabilize the positive charge through hyperconjugative effects, which are less prominent than resonance effects. Thus, the first reaction has a lower activation energy. Contrasting case D is a general chemistry example and requires the learner to consider the intermolecular forces of water and hydrogen chloride molecules.

Besides these rather theoretical tasks, contrasting cases can also be designed for practical purposes, especially when the hypothesis derived while solving a case can be tested by experiments. Thus, reasoning about the differences in a contrasting case could be the starting point of a predict-observe-explain cycle, resulting in hypothesis that are further tested in an inquiry process (White & Gunstone, 1992). Potential experimental cases should allow observations and measurement of macroscopic differences between the reaction processes, in terms of differences in color, conductivity, or pH values. Various experimental cases have already been developed (Schmitt & Schween, 2018) and can be used in the classroom to either develop, apply, or expand students' conceptual understanding (Graulich & Schween, 2018).

According to the meta-analysis of Alfieri et al. (2013) the pure provision of contrasting cases may not be sufficient to foster students' (sustained) understanding. Instead, the combination of both, contrasting cases and prompting students to explain, seems to have positive effects. When students are engaged in explaining, they seem to learn more effectively and are better able to generalize and transfer concepts to new examples (Lombrozo, 2006). Overall the greatest benefit of explanations lies in integrating previous knowledge with new knowledge and generating a connection between knowledge pieces that is more general than the phenomenon itself (Williams & Lombrozo, 2010).

Figure 1: Variations of contrasting cases (A: submicroscopic drawings; B: representations of water; C: organic reactions, D: boiling points of substances).

A ‘Resource’ perspective on student reasoning

There might be cases in which, even with a well-designed problem, students may not be engaged in explaining in detail or providing the type of reasoning that is intended. As humans are not able to activate and use all information available to them at once, it may not be surprising that students as well should be guided in what they are expected to do. Learners need to learn how to use their knowledge and might profit from a scaffold, as a guidance that supports them to reason about the necessary information and to connect multiple aspects to solve a problem. Especially, complex tasks that require inferences and consideration of multiple variables impose a high cognitive load on the learner and may thus influence students’ answering behavior. Students may not mechanically recall all their prior knowledge, but rather, depending on the situation, use or not use their knowledge or cognitive “resources”. These resources can be understood as fine-grained pieces of knowledge and beliefs that a learner can use to approach and solve a task (diSessa, 1988; Hammer, Elby, Scherr, & Redish, 2005). While learning, resources are activated, built and connected to form a complex set of ideas. With expertise, this set of ideas gets activated as a whole or as a chunk and each resource does not need to be activated consciously.

It is worth noting, that a resource a student uses in reasoning is not inherently correct or incorrect, but may be more or less productive in a context (Hammer, 2000). A resource, useful or not useful in a context, can be thought of as being ready to use, when prompted. This perspective on students’ learning acknowledges that students hold multiple coherent or incoherent ideas and thus shifts the focus to the instructional setting that cues certain resources, i.e. supports students to use their prior knowledge.

The conceptualization of learning and retrieval through the lens of Hammer’s (2000) resources framework provides us with insights on how to advance students towards successful reasoning, by paying attention to the types of prior knowledge, ideas, and beliefs students are using, productively or unproductively, and those that students are not using in their reasoning and in certain instructional situations.

Scaffolding reasoning

The conceptual resources framework has a clear implication for effective instructions: activities that help students activate and connect knowledge pieces or reflect on how they approach a task in a specific context are useful to foster their meaning making. Scaffolding students’ reasoning can be a powerful tool to meet this goal. The term “scaffolding” describes a variety of techniques and methods to guide students through a task by providing different types of prompts, designed worksheets or even structured laboratory curricula (Seery, Jones, Kew, & Mein, 2019). Reasoning scaffolds can be used in various formats, either as sentence starters, visual representations, prompts or questions, which provide students with cues what to connect and include in their explanation (Kang, Thompson, & Windschitl, 2014; Kararo, Colvin, Cooper, & Underwood, 2019) or how to approach problems (Yuriev, Naidu, Schembri, & Short, 2017). Scaffolds are commonly thought of being a temporary support that is withdrawn when the learner progressively internalizes the scaffold. Thus, scaffolds are meant as a tool to reduce the cognitive load that a complex task may impose on the learner (Kirschner, 2002; Sweller, van Merriënboer, & Paas, 1998). By temporarily supporting the problem-solving process and building up skills and abilities, a learner learns to independently solve tasks, when the scaffold is withdrawn. Scaffolds should not simplify tasks, they should as well represent the complexity inherent to a task, but prepare the learner to cope with the complexity when the scaffold is withdrawn.

Figure 2 illustrates the difference between two possible instructional situations; one is not scaffolded, the other is scaffolded. Without a scaffold, the student might use some pieces of his or her prior knowledge for an explanation, but may miss other aspects that he or she would be able to use. The reasons for not activating these pieces can be manifold, the student has missing prior knowledge or has different assumptions on what a task requires (Figure 2, left side). Independent of the underlying cause, it is difficult in this case to support the students to activate the missing resources because, without a clear understanding how the answer should be structured, it is not clear, for the learner and the teacher what type of knowledge pieces the answer should contain. In the

Figure 2: Illustration of comparing scaffolded and not scaffolded instruction.

second case, when the reasoning process of the student is scaffolded, it is clear beforehand for the teacher, how the single knowledge pieces necessary for an appropriate answer should be connected (indicated by the green line connecting the boxes, Figure 2, right side). Considering each piece can now be scaffolded through instructional prompts. It can guide students to activate knowledge resources that they would not use on their own.

Stepwise design of a reasoning scaffold

The question now arises how it is possible to derive an effective reasoning scaffold to support students in answering a specific type of problem. This can be done in several steps. The first step in this process is to 1.) define the problem type that is worth structuring for the students. Especially problems that require students to combine multiple aspects and draw inferences are best suitable for reasoning scaffolds, as they might impose a high cognitive load without scaffolding. Questions that require a simple recall of facts are not suitable for scaffolds. Second, it is important before creating prompts to 2.) define how the ideal answer would look like, what is important and what is not necessary. This ideal answer should match the level of competencies that a student is supposed to have at a certain stage of the course. It can make sense to use a scaffold at a stage where students are supposed to apply their prior knowledge to a new situation in order to support them using the appropriate knowledge and connecting it in a way that is meaningful to the new situation. It can also be useful to employ a scaffold at a stage where students are expected to generate an idea that is new to them based on the combination of prior knowledge in novel ways.

This ideal answer is then the baseline to 3.) derive a generic reasoning structure that shows how the knowledge pieces and aspects are combined in an answer. Based on this reasoning structure, instructional prompts can be created that address each component of the structure, e.g. describe, how the displayed representations are different. These prompts should guide the students through the problem, by prompting them to identify and connect the relevant pieces. In the last step, a worksheet can then be designed to visualize the process, e.g. a scaffold grid.

Defining the problem type

Every process of creating a reasoning scaffold should start with the type of problem that the teacher wants to structure for the learner. This could be a fundamental problem type common in a discipline, one that students

struggle with because of complex problem-solving steps, or one that requires considering multiple variables. For the case of organic chemistry, the main challenge for students is to consider the implicit conceptual level and to derive cause-effect relations when reasoning about multiple organic representations. This type of reasoning is often not induced by using single cases, as students tend to re-describe a given reaction rather than focusing on the underlying processes and reasons for it (DeCocq & Bhattacharyya, 2019). If we want students to be engaged in more than describing a reaction, e.g. the steps of an S_N1 reaction, a promising problem type to engage students to attend to implicit features of reaction mechanisms is to use contrasting cases, i.e. comparing two S_N1 reactions. Comparing reactions requires to consider qualitative differences of properties or effects, e.g. why is a tertiary carbocation formed faster than a secondary carbocation. Without contrasting a case to another the point of reference is missing. Additionally, deriving concepts through case comparisons has a long tradition in the discipline itself (Goodwin, 2003), as many of the well-known concepts used in organic chemistry have been derived from competitive experiments, in which only one variable has been changed (Graulich & Schween, 2018). Bartlett and Knox (1939), for instance, compared the solvolysis of two tertiary chlorides, 1-chloroapocamphane and *tert*-butyl chloride. Based on this competitive experiment, they determined that a carbocation is only formed when it can establish a planar structure. The rigid structure of the apocamphyl backbone prevents the rehybridization to a planar sp^2 -carbon, making a nucleophilic substitution impossible.

Figure 3 shows an example of a contrasting case that asks the learner to make a judgment about the relative activation energy of the two reaction steps. Both leaving group departure steps differ only in one variable, i.e. the structural difference CH_2 -group (reaction A) and adjacent double bond (reaction B). This difference, however, strongly influences the activation energy of this leaving group departure step. This example contrasting case is worth structuring with a scaffold for multiple reasons: 1) It is a problem that is very typical for the discipline of organic chemistry and thus important for students to deeply engage with. 2) The contrasting case nature of the problem gives reference points that scaffolding can build on. For example, one can ask how the double bond influences the activation energy differently than the CH_2 -group. If only reaction B would be depicted, the problem would not be as suitable for scaffolding because a prompt asking about the influence of the double bond on the activation energy would not be meaningful if there is no point of reference. 3) The problem requires the students to make inferences that are not directly depicted, e.g. about resonance effects, thus scaffolding can support students to go beyond the surface level of what is depicted and it can give guidance of what to look for beyond the surface level. 4) Making a judgment about the influence of a qualitative difference of electronic effects on the activation energy can impose a high cognitive load on the learner since it requires the consideration of implicit information, cause-effect reasoning, and reasoning about different areas of chemistry, e.g. structural vs. energetic (Caspari, Kranz, & Graulich, 2018). Scaffolding prompts can reduce this cognitive load by aiming at different portions of this complex task.

Defining the ideal problem solution

When solving the given case in Figure 3, one has to consider first what is actually different between the starting materials (differences) and what changes in this mechanistic step (similarities) in order to derive a causal argument of how the differences between the reactants might influence the process and thus influence the activation energy.

One could solve the case in the following way: “In reaction B, due to the adjacent double bond, the π -orbital of this bond can overlap with the empty p -orbital of the forming carbocation. This resonance distributes electron density in the transition state. In reaction A, the two C–H bonds can donate electron density to the empty p -orbital via hyperconjugation. The effect of resonance is stronger than the hyperconjugative effect, thus the activation energy of step B is lower.”

This answer is one possibility of an ideal problem solution for this case and should not mistakenly be considered as a student answer. It only serves the purpose of clarifying what is needed in an answer. Another argument that might not be commonly taught in the organic chemistry classroom, is to reason in the following

Which of the two reaction steps **A** or **B** has lower activation energy?

Figure 3: Example of an organic contrasting case between reaction A and reaction B (correct answer B is highlighted).

way: “Both reactions, A and B are endergonic ones and, therefore, the transition state for both reactions are late on the reaction coordinate and product-like according to Hammond’s postulate. Therefore, the more stable product (carbocation in reaction B, Figure 3) forms via the lower transition state and, thus, with lower activation energy.” This answer concludes from the difference in thermodynamic stability of the products to the transition state of the reactions. Depending on the ideal answer, the next steps, such as defining the reasoning structure and the corresponding scaffold prompts change. We will use the former ideal answer to illustrate the next steps.

Deriving a generic reasoning structure and prompts

On the basis of this ideal answer, given in the former paragraph, we need to generalize how the problem solution is formed and what type of components have been used in order to derive a more generic reasoning structure that is common to this problem type.

When we now deconstruct the ideal problem solution into reasoning pieces, one recognizes that the answer connects reasoning about structural differences (e.g. C=C- vs. CH₂-group) and changes (e.g. empty *p*-orbital forms) of the reaction step by creating a causal relation. This causal relation is created by inferring an implicit structural cause, e.g. implicit property, and using this cause to derive an (electronic) effect on the change (e.g. overlap of the π -orbital of the double bond with the empty *p*-orbital of the forming carbocation) (Caspari et al., 2018). With this relation, a causal chain (structural claim) is established that now serves as a basis to make a claim (energetic claim) about the differences in activation energy. Figure 4 shows a visualization of the generic reasoning structure that is common to answering all types of mechanistic contrasting cases, in organic chemistry or in other disciplines (Caspari & Graulich, 2019; Caspari, Kranz, & Graulich, 2018).

On the basis of this generic reasoning structure, reasoning prompts can now be formulated to guide the process of information seeking and connecting (Figure 4). For our exemplary contrasting case, as well as contrasting cases in general, it is important to prompt students to go beneath the surface of the representation and to infer implicit information, such as properties of entities (e.g. electron density). It is natural that students do not effortlessly use all their available prior knowledge as the human cognition tries to work economically (Evans, Newstead, & Byrne, 2004). Similarities on the surface are much more prominent and accessible for the learner and are, thus, used in their reasoning. Inferring implicit information, such as properties of functional

Figure 4: Generic reasoning structure for mechanistic contrasting cases and reasoning prompts.

groups, does not come easily and students need to learn that this is a required step. A scaffold can help to fulfill this job, until students are at ease with this type of reasoning.

A grid with empty boxes can be used to visually connect the aspects for the structural claim (cf. Figure 5). When using this grid, one relation connects 1.) one structural difference of the given case (i.e. What is different between the compared molecules?) and 2.) a typical change occurring in this process (i.e. What changes in the process?), by 3.) verbalizing a cause-effect relation (i.e. What influence does this difference have on change?). The boxes of the worksheet grid are connected by an arrow, referring back to the reasoning structure in Figure 4. This connection shows how reasoning about properties leads to reasoning about an effect which has an influence on the change of the process.

The worksheet grid in Figure 5 exemplarily shows how this grid can be used to solve the contrasting cases in Figure 3 (Instructional Prompt: Which of the two reactions has the lower activation energy). The first two steps to work with the grid would be to note the changes that occur in the process (e.g. the formation of the empty p -orbital of the carbocation and the formation of a negatively charged leaving group) and the structural differences (e.g. $C=C$ - and CH_2 -group). Afterward, each structural difference is related to each of the changes by describing a possible influence. It seems trivial to structure the process in smaller steps, but students tend to jump to the final answer of the question without having thought about the underlying reasons. It slows down their reasoning process and helps to collect their thoughts first.

This worksheet can be used to solve cases with either single or multiple influences. If the cases are more complex and contain multiple variables or multiple changes, the grid can be expanded. The additional step afterward is to weigh the strength of the described effects and then to connect this structural claim to the energetic claim, which is not included in this worksheet grid. It is as well possible to describe relations, in which a structural difference has no influence on the change. This helps students to identify multiple influences in a case, even though they might not be relevant. Given the perspective of the resources framework, it is important that students recognize that reasoning about an aspect might be relevant in one context, but not in another. Supporting students in multi-variate reasoning does not only require to collect all relevant influences of a contrasting case, but also the variables that have no influence.

The scaffold, as presented here, only allows to solve mechanistic contrasting cases, i.e. cases that require to reflect on a change of a process. The contrasting cases A and B, given in Figure 1, for example, are not suitable, as they are not focusing on a process and rather compare features of representations. The given cases C and D in Figure 1 are mechanistic contrasting cases, as one is required to reflect about the ongoing chemical process, i.e. the mechanism of the process. We can now easily apply the reasoning scaffold to contrasting case D: *Why does water have a boiling point at 100 and hydrogen chloride at -85 degrees Celsius* (Figure 6).

Figure 5: Scaffold grid for comparative mechanistic reasoning, exemplified for the contrasting case in Figure 3 (correct answer B is highlighted for the reader).

Figure 6: Solving a general chemistry contrasting case with the scaffold.

The first step is to identify the differences between the molecules (submicroscopic level) of the two substances (macroscopic level) and to reflect on the change of the process, e.g. decrease of intermolecular interactions in the process of boiling. Multiple influences can then be derived that influence the process of boiling. When using the scaffold for this contrasting case, it becomes evident that more than only one influence impacts the boiling process of water compared to hydrogen chloride. Although one would be satisfied if students would mention the stronger intermolecular forces of water molecules as the cause of this boiling point difference, the scaffold helps to reason about multiple causes and highlights that it is not only a single influence, for example the difference in electronegativity.

Applying the reasoning scaffold with students in organic chemistry

The scaffold grid as shown in the former paragraphs and highlighted in Figure 5 allows students to infer implicit information of representations and reason about the influence on changes in a mechanistic process. As such, it provides a helpful tool for supporting students' mechanistic reasoning. In addition to the design of the scaffold, we were interested in how students are using and working with this scaffold and if it changed their answering behavior when solving complex contrasting cases (Caspari & Graulich, 2019).

We used the reasoning scaffold shown in Figure 5 and analyzed how students used the scaffold and compared students' reasoning without and with the scaffold in an interview setting. 20 undergraduate chemistry and food chemistry students from an Organic Chemistry II (OC II) course at a German university took part in the study. In the first part of the interview, students were asked to think aloud about two mechanistic contrasting cases (Figure 7). For both problems, students were asked to predict for which of the two reactants the represented leaving group departure step has lower activation energy. After solving both problems by themselves while thinking aloud, the students were asked to solve the same problems again, this time with the reasoning scaffold.

Both problems are designed as complex contrasting cases, thus each problem has two structural differences (in gray) and at least three valid variables that influence the activation energy. In problem 1, the reactants exhibit different influences in the mechanistic step, i.e. C=O-group (electron-withdrawing effect), C=C-group (electron-donating effect) and CH_3 -group (electron-donating effect). The electron-donating effect of the methyl group relies on hyperconjugation, whereas the electron-donating effect of the double bond relies on resonance. In problem 2, the reactants differ in terms of the *t*-butyl group (relief of electronic repulsion), the

Prompt: Predict for which of the two reactants the represented mechanistic step has lower activation energy.

Figure 7: Problems used in the study (explicit differences are encircled in gray, correct answers are given, B for problem 1, and A for problem 2).

CH_3 -groups (electron donating effects) and the leaving group Br/Cl (accommodation of negative charge). These structural differences have competing influences. Additionally, some of the influences are unfamiliar to the students, at least in the context of substitution reactions. The carbonyl function with its electron-withdrawing ability was known to the study participants, but its influence on the departure of a leaving group had not been discussed in class. When designing the problems, we aimed at this complexity, so that students are not able to solve the cases by recalling memorized facts. We wanted to prompt them beyond their course knowledge, to investigate how students make sense, when confronted with unfamiliar influences. We believe that the considerations we had when designing the contrasting cases for our interview study can serve as example considerations for educators when designing problems to use in combination with a scaffold for in-class activities. It is important to have clear expectations about what thinking steps the problem requires and how these relate to previous coursework the students were engaged in.

How was the scaffold used and did it help students?

During the interview, the students did obtain the scaffold grid, as exemplarily shown in Figure 8, and the prompts for each box by the interviewer (cf. Figure 5). No additional prompts other than clarification questions about what a student meant with a particular statement were used besides those of the scaffold.

The interview situation in which this data was collected is not directly comparable to an in-class situation as it was a single one-on-one interview involving the interviewer and a student, but the scaffold could be used in similar ways in different in-class settings. For example, the scaffold could be used by the educator to elicit reasoning from multiple students in a whole class discussion. After an introduction into how the scaffold works, the scaffold could also be used by groups of students to collaboratively work on problems. Figure 8 shows how one participant, Fabian (pseudonym), filled out the scaffolding grid for problem 2. We choose Fabian's scaffolded reasoning as an example of how students were guided through and worked with the scaffolding worksheet. A similar process could be used by educators when working with scaffolds like this. First, the interviewer asked Fabian to list all the changes that he sees occurring in both mechanistic steps. Fabian listed "steric," "charge," and "entropy" and explained what he meant with those key words. For example, he explained that the central carbon changes from sp^3 to sp^2 and thus from an angle of 109.5° – 120° . Then, the interviewer asked Fabian to list the differences he can see between the two molecules and Fabian made note in the respective cells of the grid and explained how he sees those differences in the mechanistic representation. For example, when writing the words isobutyl and methyl he pointed at the *tert*-butyl and the

Figure 8: Exemplary worksheet of a student, correct answer A is highlighted for the reader. Parts of the scaffold reproduced with permission from reference (Caspari & Graulich, 2019). Copyright 2019, ISER The International Society of Educational Research. Printed under a Creative Commons Attribution 4.0 International license.

Figure 9: Numbers of students who employed the given number of influences when solving problem 1 and 2.

methyl group on the worksheet. For each combination of difference and change, e.g. difference 1 and change 1, the interviewer then rephrased what the student had written and asked what influence the difference has on the change. For example, the interviewer asked questions like the following one: What influence do those two different groups you pointed out (pointing on *tert*-butyl and methyl group) have on this steric change that you mentioned? Fabian then filled in key words in the cell for influence A and explained his reasoning that if isobutyl (he means *tert*-butyl) is bulkier than methyl, then the additional space it gains through the change from 109.5–120° in the process leads to a greater gain in energy. In this manner, the interviewer and Fabian walked through the entire grid and Fabian explained additional influences, i.e. influence C and D, and also discovered that sometimes a difference has no influence on the change, e.g. influence B. For example, Fabian explained that none of the differences has any influence on the change in entropy that occurs because one molecule dissociates into two ions. It is important for students to realize that some lines of thought like the entropy change are not ignored for arbitrary reasons but need to be considered and then intentionally dropped if there is no influence of the differences between the molecules on the entropy change.

To examine the effect of the scaffold, we compared how students' use of influences changed from solving the cases without to solving them with the scaffold (Caspari & Graulich, 2019). Implicit influences that students connected with explicit differences and changes were coded. Codes were given for implicit influences typically discussed in organic chemistry classes, e.g. electron-donating effect. We compared student individual improvements when working with and without the scaffold, by using a paired-samples *t*-test. The students significantly connected more implicit influences with explicit differences and change with the scaffold ($p < 0.001$), and the increase has a large effect size (Cohen's $d = 1.272$). Figure 9 demonstrates how many students reasoned about a certain number of influences.

We found that for problem 1, with the scaffold, fewer students considered only one or two implicit influences, and more students considered three implicit influences. For problem 2, we saw that fewer students considered zero or only one implicit influence and more students considered two or three implicit influences. Thus, the presence of the scaffolding prompts led students to connect more implicit influences with explicit differences and change, which means they were accessing prior knowledge and could use and connect their knowledge to reason about additional influences, about which they did not reason on their own without the scaffold.

In our research study, we have not investigated if and to what extent the scaffold gets permanently integrated into students' reasoning, and how sustainably the scaffold influences student answering patterns in future cases. This will be subject of future research. What we could observe, though, was that while the interviewer had to explicitly give each scaffolding prompt when the students worked on the first problem, multiple students used the grid to walk themselves through the problem-solving process when working on the second problem. This is promising for practice since it indicates that students might quickly internalize the reasoning structure and employ it by themselves, which would be the ultimate goal of the use of the scaffold in practice.

Conclusion

Reasoning scaffolds can be manifold in nature and, depending on the context, are suitable tools to support students in their reasoning, when they are calibrated to a student's current level of knowledge and abilities and

help the student accomplish tasks that he or she could not accomplish alone. When considering this definition, the explicit development of a scaffold demands two central aspects from the educator. On the one hand, it reminds us of being clear about what we expect from a student, when solving a task, e.g. how should an answer look like. One needs to reflect on 1.) the complexity of and 2.) the depth of the explanation required. On the other hand, it also reminds us to anticipate the steps that a learner has to undergo to achieve this answer. The educator may not always be explicitly aware of these aspects, and thus they might not be transparent for the student. The effort for developing a scaffold is valuable not only for the students, who get a tailored support, but also for educators. Educators can use the scaffold and students' use of it as a diagnostic tool. Observing students while working with a scaffold, provides insights about the activated resources (Broman & Parchmann, 2014).

However, reasoning scaffolds are not an all-in-one device. First of all, while the reasoning scaffold improved students' reasoning about multiple influences, weighing these influences was very difficult for the students in our cohort. They were missing experience or experimental data to decide which influences to give more weight. This is expressed by Yannick: *I think by doing it in small steps, looking at the task, then some things become apparent, always more things that were not apparent when just looking at it quickly. [...] But you get into ... I think you get into this predicament, then, where you have to weigh ... Because then you have this effect and that effect. [...] And then I'm stuck anyhow.*

The reasoning scaffold, presented herein, focuses on supporting students to generate and collect multiple arguments when solving mechanistic contrasting cases. The act of weighing these arguments is not scaffolded by the grid in Figure 5 and students need further support either in the classroom or by providing additional information, e.g. kinetic data about reaction rate, to make a sound decision.

Secondly, a reasoning scaffold should be adapted to students' abilities and their prior knowledge. If a scaffold is too highly structured, it may become an algorithm, if it is too ill-defined, it may not meet the intended purpose and does not activate the necessary resources in students' reasoning. Thirdly, students might struggle at the beginning, when confronted with unfamiliar instructional prompts. In our case, inferring and describing properties of entities, e.g. the electron-withdrawing ability of a carbonyl function, was easier for the students than verbalizing the effect on the change. In this case, students can be supported additionally by a language scaffold, a fill-in-the-blanks text, or by worked examples on how to answer the prompts. Fourthly, the more a reasoning scaffold allows a generic application to multiple cases, the more students can get used to it and become familiar with the reasoning steps. Then, at some point in the learning process, when the reasoning steps are internalized, i.e. a complex set of ideas and strategies is established, the scaffold needs to be withdrawn. This act of fading the scaffold is important to transfer the responsibility back to the student.

The presented reasoning scaffold for solving comparative cases provides a scaffold that not only is applicable to organic chemistry education but to any type of mechanistic case comparisons.

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