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Scaffolding the structure of organic chemistry students' multivariate comparative mechanistic reasoning

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Abstract
Problem solving in all sciences requires the integration of multiple causal variables. Organic chemistry students often limit their reasoning about multivariate mechanism problems to single variables. To our knowledge, no teaching instrument that uses the structure of mechanistic reasoning to explicitly foster the consideration of multiple variables has been empirically evaluated to date. To fill this gap, we developed a scaffold based on findings in philosophy of organic chemistry and tested it in a qualitative interview setting. The scaffold provides a stepwise reasoning structure to compare the activation energy required for two different molecules to undergo the same type of mechanistic step. We found that the scaffold builds on what students already do when engaging in comparative mechanistic reasoning by themselves and supports their multivariate reasoning. The applicability of the structure of the scaffold in other contexts of mechanistic reasoning including physics is discussed.

Keywords
Mechanistic reasoning, multivariate reasoning, philosophy of organic chemistry, reasoning structure, scaffold

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Introduction
Central to predicting complex phenomena is the integration of multiple causal variables. While considering multiple causal variables is important for students who are reasoning about phenomena in their everyday world, multivariate reasoning is also fundamental to scientific discourse in research and in science classes.

People often limit their reasoning about complex phenomena to fewer than the total number of causal variables (Gigerenzer & Gaissmaier, 2011; Kuhn, 2007; Kuhn, Iordanou, Pease, & Wirkala, 2008; Kuhn, Ramsey, & Arvidsson, 2015; Todd & Gigerenzer, 2000). In Kuhn et al.'s (2015) study, lay adults' most frequent choice for predicting an everyday phenomenon was use of a single cause, even though multiple causal variables had been explicitly introduced to them.

Organic chemical reactions are complex systems composed of multiple variables; therefore, predicting the mechanisms of those reactions requires multivariate reasoning (Kraft, Strickland, & Bhattacharyya, 2010). When reasoning about mechanisms, organic chemistry students must not only integrate given variables but also infer implicit variables that are not explicitly shown in mechanistic representations (Bhattacharyya & Bodner, 2005; Ferguson & Bodner, 2008; Grove, Cooper, & Rush, 2012; Strickland, Kraft, & Bhattacharyya, 2010; Weinrich & Sevian, 2017). Thus, mechanistic reasoning in organic chemistry, i.e. multivariate reasoning, is very difficult for students.

As in other fields of chemistry (Furió, Calatayud, Bárcenas, & Padilla, 2000; Maeyer & Talanquer, 2013; Rozier & Viennot, 1991), organic chemistry students often rely on one variable when solving complex problems (Bhattacharyya, 2006, 2014; Kraft et al., 2010). One example is that students predict the acidity of organic molecules solely as a function of bond polarity, i.e. a single variable (Bhattacharyya, 2006). Students also tend to limit their reasoning about the reactivity of polyfunctional molecules to one functional group (Bhattacharyya, 2014).

While the confinement of student reasoning to a single variable is reported in many instances, not much is known about teaching approaches designed to foster student multivariate reasoning. In two multi-lesson interventions, Kuhn et al. (2015) provided middle school students with educational software that uses graphical representations to explore the effects of multiple

State of the literature

- Students often use one-reason decision making when multivariate reasoning about mechanisms is required.
- Scaffolding is an effective tool for helping students to engage in more complex reasoning, however, no scaffold that relies on the structure of mechanistic reasoning has been investigated to date.
- Information about the structure of mechanistic reasoning can be found in philosophy of organic chemistry.

Contribution of this paper to the literature

- We used information from philosophy of organic chemistry to develop a general structure of comparative mechanistic reasoning. This structure provided the theoretical basis for design of a scaffold thought to support students' multivariate mechanistic reasoning.
- Our qualitative interview study demonstrates that the scaffold builds on what students already do when solving comparative mechanism problems by themselves.
- The scaffold supported participants in identifying more implicit influences than they identified without scaffolding.

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variables on everyday phenomena such as obesity. After the interventions, significantly more students of the intervention groups engaged in multivariate reasoning than students of the control groups (Kuhn et al., 2015). Another approach to foster student reasoning about complex problems is scaffolding. Broman, Bernholt, and Parchman (2018) investigated to what extent scaffolding is effective in supporting complex reasoning about context-based chemistry problems. Using the Model of Hierarchical Complexity (Bernholt & Parchmann, 2011; Broman, Bernholt, & Parchmann, 2015) and the idea of stepped supporting tools (Fach, de Boer, & Parchmann, 2007), Broman, in an interview setting, asked students to solve complex chemistry problems by themselves before she provided predefined hints intended to support them in reaching a higher level of complexity (Broman et al., 2018). Hints including three types of operators were given to the students: *Name* was intended to focus students' attention on functional groups, *describe* was intended to support students in describing processes, and *explain* was intended to cause students to think about uni- and multivariate causality. Broman gave the concrete hints verbally and in individual response to what a student said about the specific problem at hand. This type of scaffolding led to an increase in students' complexity of reasoning including the multivariate aspect. However, scaffolding of this type depends on an interviewer, teacher, or more proficient peer who informs the learner about what to *name*, *describe,* and *explain* in the context of the specific problem. Since Broman et al.'s (2018) type of scaffolding only provides learners with transferable actions but not with transferable information about how to include content in these actions, learners might experience difficulties transferring the process to other problem contexts. For mechanistic reasoning, information about how to include content in the reasoning process can be provided when scaffolding builds on mechanistic theory about (1) general aspects of mechanistic reasoning and (2) how these aspects are structurally connected. Scaffolding always depends on a more knowledgeable other (Vygotsky, 1978), but in the case of scaffolding that builds on mechanistic theory, the support is fully included in the tool used for scaffolding, i.e. the scaffold. Hence, solving a process with the scaffold does not depend on a more knowledgeable other's reasoning about the concrete problem at hand, and transfer to other contexts should be facilitated. Our development of such a supporting tool was, thus, guided by theory about the structural connection of aspects of mechanistic reasoning.

Theoretical Framework

Talanquer and coworkers describe key aspects of mechanistic reasoning in chemistry (Sevian & Talanquer, 2014; Weinrich & Talanquer, 2016):

- explicit and implicit properties
- dynamics
- causes and effects
- multiple variables
- a complex interplay of the aforementioned aspects

This goes in line with the characterization of causal mechanistic reasoning by other researchers, who specifically focus on the aspects dynamics (how something happens) and causes (why something happens) (Becker, Noyes, & Cooper, 2016; Cooper, Kouyoumdjian, & Underwood, 2016). In addition to using key aspects to describe mechanistic reasoning, one can use the general structure of an argument (Toulmin, 1958) to describe the structure of mechanistic reasoning, as has been shown for physical chemistry (Moon, Stanford, Cole, & Towns, 2016) and organic chemistry (Cruz-Ramírez de Arellano & Towns, 2014). In contrast to Berland and Reiser's (2009) findings that point out the usefulness of the argumentation pattern for prompting students to engage in complex reasoning, Moon et al. (2016) found that students could construct complete arguments without using key aspects of mechanistic reasoning. Hence, the general structure of an argument does not necessarily help students to use aspects of mechanistic reasoning, and information about the structural connection of aspects of mechanistic reasoning is needed. With the goal to provide researchers and educators a tool to analyze students' mechanistic reasoning, Moreira, Marzabal, and Talanquer (2018) recently described 15 different patterns that a group of students used to connect aspects of mechanistic reasoning in response to one question. While this diversity of patterns served these researchers' goal, our goal to develop a scaffold requires a single, well-defined way to connect aspects of mechanistic reasoning. This is why we focused on one type of mechanistic reasoning, i.e. comparative mechanistic reasoning, which is important in the epistemic practice of organic chemistry (Goodwin, 2003). For the development of a scaffold to foster multivariate comparative mechanistic reasoning in organic chemistry, we draw from theoretical considerations of Goodwin (2003, 2008) in the philosophy of organic chemistry literature. In accordance with Talanquer's (2018) work on reasoning of chemistry experts, we do not differentiate between mechanistic reasoning used to construct an explanation and mechanistic reasoning used to construct an argument but view mechanistic rationale as referring "to any product of reasoning that uses chemical knowledge to build explanations, justifications or arguments" (Talanquer, 2018, p. 1874). We demonstrate that the structural connection of mechanistic aspects in comparative mechanistic reasoning is the same for the construction of an argument and the construction of an explanation.

Goodwin (2003) explains that mechanistic reasoning used to answer typical questions in organic chemistry is a comparative process. For example, one considers which of two reactions occurs faster or whether a reaction proceeds by one pathway or another (Goodwin, 2003). Similarities and differences of mechanistic comparisons provide important anchors for the structural connection of mechanistic aspects in comparative mechanistic reasoning.

To demonstrate this, we use the following example question of the type described by Goodwin (2003) to be typical in organic chemistry: Which electrophilic aromatic substitution in **Figure 1** is faster? Because the first step of an electrophilic aromatic substitution is rate determining, the following analysis of the structure of the comparison focuses only on the first step of the reaction. While the direct answer to the question is a claim about activation energy, information about energy is not directly accessible and needs to be inferred from the information provided by the structural formulas (Goodwin, 2003, 2008).

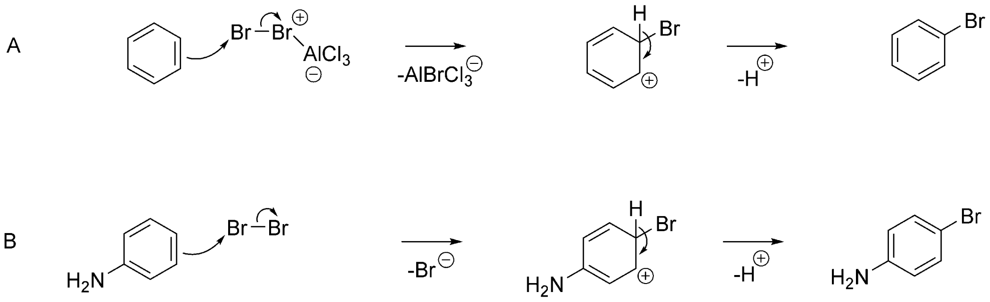


Figure 1. Comparison of the bromination of two different benzene derivates (benzene and aniline) with and without $AlCl_3$ catalyst via electrophilic aromatic substitution.

Several implicit influences that affect the activation energy can be inferred from explicit features of the structural formulas:

(1) Compared to B the $AlCl_3$ catalyst in A lowers the energy of the σ* orbital of the Br-Br bond (lowest unoccupied molecular orbital). This is a rationale for A having a greater interaction between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and, thus, a lower activation energy than B.

(2) The amino group of aniline in B donates electrons by conjugation and, thus, compared to A, increases the electron density of the π system and the energy of the HOMO. This is a rationale for B having a greater HOMO-LUMO interaction and a lower activation energy than A.

(3) The effect of electron donation by conjugation of the amino group in B can also be explained as stabilization of the positive charge that is forming in the transition state (whose structure, according to Hammond's postulate, resembles the intermediate product).

We see an identical structural connection of aspects of mechanistic reasoning in these types of rationales, namely that a relation is formed between one explicit difference of the structural formulas and a change that occurs in every electrophilic aromatic substitution, i.e. a similarity between the compared cases (**Figure 2**). The explicit difference utilized in rationale (1) is the presence of $AlCl_3$ in A, which is absent in B. The explicit difference used in rationales (2) and (3) is the presence of the amino group in B, which is absent in A. The changes that occur in every electrophilic aromatic substitution are the interaction of the HOMO of an aromatic system with the LUMO of an electrophile utilized in (1) and (2) and formation of positive charge in the transition state in (3). The structural connection between these aspects is applicable for any comparison of different molecules undergoing the same type of mechanistic step.

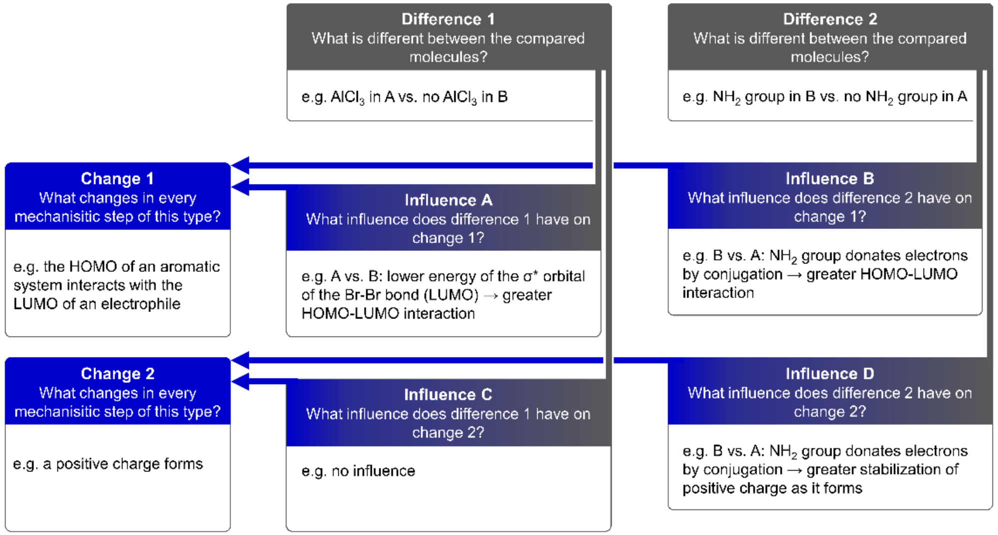


Figure 2. Structure of comparative mechanistic reasoning to answer the question *which mechanistic step is faster?* The example refers to the comparison of the two reactions in Figure 1. The number of differences, changes, and influences displayed in this figure only pertains to that example. HOMO = highest occupied molecular orbital, LUMO = lowest unoccupied molecular orbital.

The structure can be used to systematically infer multiple implicit influences in comparative mechanistic reasoning (**Figure 2**). One can independently think about changes that occur in all mechanistic steps of the represented type (**Figure 2**, changes 1-2) and explicit differences between the molecules of the two reactions (**Figure 2**, differences 1-2). Explicit differences and changes can then serve as starting and end points to infer implicit influences (**Figure 2**, influences A-D). For each combination of explicit difference and change, one may ask what influence does the difference have on the change? **Figure 2** demonstrates that the three rationales mentioned before give the answers to those questions (influences A, B, D), and that in the fourth combination the explicit difference does not have an influence on the change (influence C).

The structure represented in **Figure 2** connects the aspects of mechanistic reasoning described in the chemistry education literature (Sevian & Talanquer, 2014; Weinrich & Talanquer, 2016) in one defined way. Explicit properties that differ between the compared cases and changes, i.e. dynamic parts of mechanisms, serve as starting and end points of the reasoning structure. Reasoning about influences of the explicit differences on the changes means reasoning about implicit properties and the effects of those causes on the changes. Multiple variables are considered in terms of influences on changes, and their complex interplay is structurally organized (see **Figure 2**).

While data, warrant, and claim of an argument can contain these aspects of mechanistic reasoning, but do not necessarily do so (Moon et al., 2016), this specific structure of comparative mechanistic reasoning connects aspects of mechanistic reasoning. Furthermore, the same structural connection of aspects of mechanistic reasoning used to construct the example arguments provided before can be employed to construct an explanation. For example, if one wants to explain why an electrophilic aromatic substitution of aniline is faster than that of benzene, one can use the same influence of an explicit difference on a change, as provided in argument (3) in response to the question of which mechanistic step is faster.

To answer the question of whether reaction A or B is faster (**Figure 1**), one needs to weigh the different influences. Appropriately weighing these influences requires identifying all of them beforehand and using additional information that cannot be inferred from the structural formulas, e.g. experimental data (Goodwin, 2003). Hence, identifying influences is a cognitive task different from weighing them and is the essential basis of comparative mechanistic reasoning. This is why our study focuses on scaffolding the identification process of multiple influences by using the presented structure of comparative mechanistic reasoning.

Goals and research questions

We hypothesize that the aforementioned reasoning structure can be used as a scaffold to support students' multivariate comparative mechanistic reasoning. To be beneficial for students, the scaffold should build on the reasoning structure that students already use without the scaffold, and it should lead to the identification of more influences. It is important to build on the reasoning structure that students already use without the scaffold to activate resources that they have, which is the cognitive state in which learning can occur (Hammer, Elby, Scherr, & Redish, 2005). Furthermore, if the scaffold provides a reasoning structure that does not resemble the students' previous reasoning structure, the usage of the scaffold would be counterintuitive. Hence, this study was guided by the following research questions:

(1) To what extent does the reasoning structure provided by the scaffold build on what students already do without the scaffold? For this question the following sub-questions were explored:

  (a) Without the scaffold, to what extent do students communicate implicit influences in the theoretically proposed reasoning structure?

  (b) To what extent do students incorporate the implicit influences they identified without the scaffold into the structure of the scaffold?

(2) To what extent do students identify additional implicit influences with the scaffold compared to their reasoning without the scaffold?

Methodology

Our study was exploratory in nature because it has not been investigated before whether the structure of mechanistic reasoning described in the theoretical framework can be found in student reasoning. Furthermore, the scaffold was unknown to students and had to be introduced to them. Hence, a qualitative interview setting was most suitable to obtain answers to our research questions.

Context and participants. Interviews were conducted with 20 undergraduate chemistry and food chemistry majors in spring 2017. The sample was recruited on a voluntary basis from the Organic Chemistry II (OC II) course of a German university, which uses a traditional curriculum for organic chemistry courses. Recruiting participants via announcement in lecture and via email was stopped when a sample size of 20 students, typical for qualitative studies, was reached. 11 female and 9 male students took part in the study. They were between 19 and 27 years old. A leaving group departure step, i.e. the mechanistic example we chose for this study, was part of multistep mechanisms in the OC II course and was introduced to the students in their previous OC I course as the first step of S_N1 and E1 reactions. These reaction types were part of the OC I exam, for which the participants obtained an average course grade of 11 with a range from 5 to 15 (5 being the grade necessary to pass the exam and 15 being the best grade in the German grading system). To protect the students' identities, they are given pseudonyms. All participants were asked to give their consent for the use of their data, including their written work, for research purpose and publication. Interviews were conducted in German and student interview excerpts and written work were translated for this publication.

Problem design. The two mechanism problems used in the study (**Figure 3**) were designed as case comparisons because we wanted to investigate students' comparative mechanistic reasoning. Furthermore, based on research outside of organic chemistry about the effectiveness of case comparisons (cf. Alfieri, Nokes-Malach, & Schunn, 2013), deeper insight into students' reasoning could be expected compared to using other approaches like single cases. For each case comparison, students were asked to develop a hypothesis about which of the two reactants has lower activation energy for the represented mechanistic step, i.e. a question of the type described by Goodwin (2003) to be typical in organic chemistry. A leaving group departure step was chosen as the example for its relative simplicity but representative nature as a mechanistic scenario. It is a relatively simple—if not the simplest—mechanistic scenario because it is a single mechanistic step that involves only one reactant and the movement of one electron pair. Still, it is representative because it involves typical changes of organic mechanisms, which are changes in bonding, charge distribution, molecular geometry, and degrees of freedom. The contrasted reactants of the mechanism problems were designed so that the structural formulas differed by more than one explicit feature with the aim of encouraging multivariate reasoning.

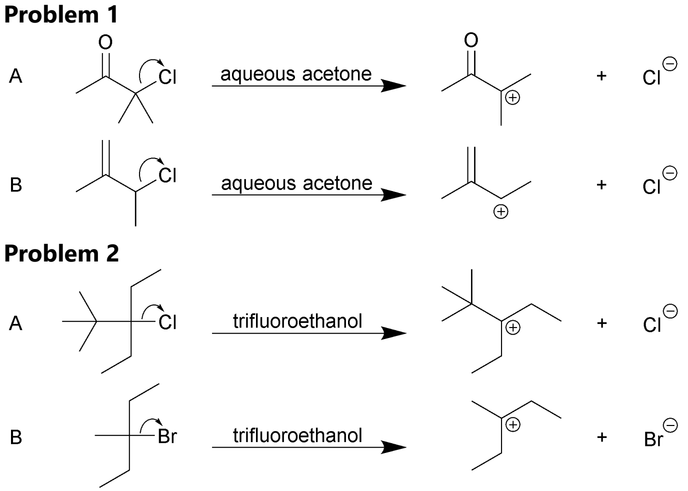


Figure 3. Mechanism problems used during student interviews. Students were asked to predict for which of the two reactants in problem 1 and 2 the represented mechanistic step has lower activation energy.

Table 1 demonstrates which influences were embedded in the problem design and why they are relevant for a hypothesis about activation energy. **Table 1** also presents information about how each influence relates to students' coursework. This information was obtained from consultation with the professors teaching OC I and II. For each problem, the same solvent was used for both cases (**Figure 3**) to simplify the comparison for the students. Due to the fact that the solvent was the same in both cases, it did not need to be and, in fact, was not considered to be an influential factor by any student and is thus not incorporated in the analysis.

Interview procedure. Semi-structured think-aloud interviews (conducted by the first author) were used to gain insight into students' reasoning processes while they were solving the mechanism problems. During the interviews, students' verbalized reasoning and their writing were recorded simultaneously with a LiveScribe pen. In the first part of the interview, students were asked to solve both mechanism problems without scaffolding. To answer research question 1a, it was important that all students answered both mechanism problems by themselves before being introduced to the scaffold because otherwise their personal reasoning structure could have been influenced by the scaffold. It is interesting for future work whether the scaffold has immediate benefits for students' self-regulated problem solving processes and whether these endure, however, this different study design would have contradicted the purpose of our study. After letting the students solve both problems by themselves, they were introduced to the scaffold by the interviewer and asked to solve the same two mechanism problems again with help of the scaffold. All participants were asked to solve problem 1 before problem 2 because we wanted all students to start with the problem that requires less transfer effort. Problem 1 requires

Table 1. Information about influences (of differences on changes) embedded in the problem design regarding the chemistry behind it and the coursework of the study participants.

Influences	Rationale for why the influence affects the activation energy[A]	Relation of the influence to students' coursework
Problem 1		
Electron donation of the additional methyl group in 1A	• Stabilizes the positive charge of the carbocation • Positive charge is already partially formed in the transition state → Influence lowers the activation energy	• Influence was taught to the students in the context of the mechanistic step used in the study • Influence is explained to be caused by hyperconjugation and induction in the students' textbook (Buddrus & Schmidt, 2015) → both explanations are deemed plausible
Delocalization of the π electrons of the C=C double bond in 1B	• Stabilizes the positive charge of the carbocation • Positive charge is already partially formed in the transition state → Influence lowers the activation energy	• Influence was taught to the students in the context of the mechanistic step used in the study
Electron withdrawal toward the carbonyl oxygen in 1A	• Leads to a partial positive charge at the carbonyl carbon that electrostatically repels the positive charge of the carbocation • Positive charge is already partially formed in the transition state → Influence raises the activation energy	• Influence was taught to the students, but not in the context of the mechanistic step used in the study • This is because infeasible mechanistic steps are not usually considered in traditional curricula
Problem 2		
Electron donation of the *tert*-butyl group in 2A	• Stabilizes the positive charge of the carbocation • Positive charge is already partially formed in the transition state → Influence lowers the activation energy	• Influence was taught to the students in the context of the mechanistic step used in the study
Greater capacity of Br to accommodate negative charge in 2B	• Due to its larger size, Br has a greater capacity to accommodate negative charge than Cl • Negative charge on the leaving group is already partially formed in the transition state → Influence lowers the activation energy	• Influence was taught to the students in the context of the mechanistic step used in the study
Greater relief of B-strain in 2A	• Due to the more bulky *tert*-butyl group in 2A, the relief of B-strain (relief of electron repulsion between substituents) that accompanies the widening of the bond angle during the change from sp^3 to sp^2 hybridization is greater (Liu, Hou, & Tsao, 1998, 2009; Smith, 2013) → Influence lowers the activation energy	• Influence was not taught to the students

[A] The rationales given are only one way to explain why the influences affect the activation energy. The influences can be explained in multiple different ways.

less transfer effort because, in problem 2, an influence was embedded that was entirely unknown to the students based on their coursework, i.e. the relief of B-strain (**Table 1**). During the interviews, follow-up questions were used to ensure that students connected terminology they used with the underlying meaning. If a student explained a term, e.g. +I effect, in the first part of the interview and referred to it again in the second part of the interview, the student was not asked to explain the same term again because it could be assumed that the student implied the same meaning.

Scaffolding. The instructional steps of the scaffolding process are based on the theoretically proposed reasoning structure that we developed on the basis of philosophy of organic chemistry. At the same time, the scaffold follows the principles of cognitive load theory (Sweller, 1994; van Merrienboer, Kirschner, & Kester, 2003) by taking into account this general "structure of information and the cognitive architecture that allows learners to process that information" (Paas, Renkl, & Sweller, 2003, p. 1). Hence, instructions for the second part of the interview were designed so that the students could develop the complex reasoning structure stepwise. All instructional steps were explained to the students verbally by the interviewer and in a written format (**Appendix**). For making notes, the students were provided with several tables like the one shown in **Table 2**. The first step of the scaffold was to list all changes happening during a leaving group departure step (**Table 2**, left column). The second step was to list all explicit differences between the contrasted molecules (**Table 2**, top row). The third instructional step was to explain how the differences influence the changes (**Table 2**, intersections of differences and property changes). We expected students to identify implicit influences, which were the focus of our study, in response to this instruction. The students were told that the problem solving processes are not limited to a certain number of changes, differences, and influences. The fourth instructional step was to use the information collected in the steps before to form a hypothesis about which of the two reactants undergoes the leaving group departure step with lower activation energy. This step was only thought to round out the interview for the students, and their reasoning in this fourth step was not part of the analysis, as our study focused on the identification of multiple influences and not on the quality of students' final claims.

Analysis. The interviews were transcribed verbatim. The qualitative analysis was performed using the coding software MAXQDA. Implicit influences used by the students in their problem solving processes were coded. Codes were given for plausible influences that could be expected based on the problem design (**Table 1**) and for influences that were not plausible based on the problem design but were prevalent in students' reasoning. Constant comparison (Corbin & Strauss, 2015) was used to categorize the influences used by the students. Since we were interested in identifying frequently used influences, those that were mentioned by two or fewer students were categorized as infrequent influences and were only of interest for the number of influences a student used. Moreover, we coded whether the influences that students employed in their initial problem solving processes (without the scaffold) were communicated in the theoretically proposed reasoning structure, i.e. we decided whether an influence was used to construct a relation between an explicit difference and a change. The first author (PhD candidate with a master's degree in chemistry education) coded the entire data set in constant reflection with the second author (chemistry education professor). For interrater reliability, the second author independently coded 20 percent of the data. Discussion between the two researchers led to full interrater agreement that faithfully represents the data. An in-depth analysis of students' initial reasoning in the first part of the interviews performed to answer different research questions is the subject of another publication (Caspari, Kranz & Graulich, 2018).

Table 2. This table reflects the scaffolding process and was provided to the participants during the second part of the interviews so that they could use it to make notes. In the scaffolding process, students were asked (1) to identify all property changes (left column), (2) to identify all differences (top row), and (3) to explain all influences (intersections of differences and property changes).

	Difference 1 *atom or group of atoms difference between A and B?* space for students' entries	Difference 2 *atom or group of atoms difference between A and B?* space for students' entries
Property change 1 *property change of the reactant that increases or decreases the energy of the reactant?* space for students' entries	Influence A *influence of the difference (above) on the property change (left) / effect on the change in energy?* space for students' entries	Influence B *influence of the difference (above) on the property change (left) / effect on the change in energy?* space for students' entries
Property change 2 *property change of the reactant that increases or decreases the energy of the reactant?* space for students' entries	Influence C *influence of the difference (above) on the property change (left) / effect on the change in energy?* space for students' entries	Influence D *influence of the difference (above) on the property change (left) / effect on the change in energy?* space for students' entries

Results

Although the students did not yet know the scaffold during their initial reasoning processes, they communicated all influences that they considered in the theoretically proposed reasoning structure on which the scaffold is based. **Table 3** shows all frequently used influences that each student identified in their initial processes of solving problem 1 and 2 and demonstrates that all of these influences were used to describe an influence of an explicit difference on a change (**Table 3**, green cells). For example, Marie considered one influence in her initial process of solving problem 1, i.e. electron donation of the additional methyl group in 1A, and communicated it in the theoretically proposed reasoning structure:

> Marie: *Well… for that, I would now look at the carbon at which the reaction or the step happens. And we have a tertiary carbon in A, and here [in B] we have the secondary. […] And this has effects on how the carbocation formed is stabilized. […] Well, in A we have two methyl substituents and in B there's only one. […] And the methyl substituent has a positive inductive effect. And that means it's electron-donating, and that's why we can stabilize the positive charge. And, well, in A we have two of these methyl substituents and in B there's only one. That means, because of that, I would say that A has the lower activation energy.*

The excerpt demonstrates that Marie used electron donation via induction to describe an influence of the explicit difference tertiary vs. secondary on a change that occurs in every leaving group departure step, i.e. the positive charge of the carbocation that is only present in the product and not in the reactant of the mechanistic step.

The fact that all students communicated influences in the theoretically proposed reasoning structure when they were solving the problems by themselves is an indication that the scaffold builds on what students already do without the scaffold.

Moreover, from 55 frequently used influences that the 20 students identified when solving the two problems by themselves (in the first part of the interview), they incorporated 54 into the structure of the scaffold (in the second part of the interview), another indication that the scaffold builds on what students already do without its support (**Table 3**, green cells). This is demonstrated by Marie's entries in the table provided to her during the second part of her interview (**Table 4**). Like in her initial reasoning process, she connected the explicit difference tertiary vs. secondary (**Table 4**, difference 1) with the change of positive charge formation (**Table 4**, property change 1) by making a note about the +I effect in the cell for influence A (**Table 4**, intersection of difference 1 and property change 1).

In addition to these two indications that the scaffold builds on what students already do without the scaffold, we found that 20 of 40 problem solutions already contained multivariate reasoning (i.e. two or more influences) without help of the scaffold (**Table 5**). Additionally, the multivariate problem solutions increased to 31 of 40 with support of the scaffold (**Table 5**). For at least one of the two problems, 15 students identified more influences with the scaffold than they did when solving the problems by themselves (**Table 5**). While the scaffold did not support all students in considering more influences, case comparisons in combination with the scaffold led to a high level of multivariate reasoning.

While Marie only identified one influence when solving problem 1 by herself, she identified an additional influence with support of the scaffold. The scaffold guided her to reason not only about an influence of the additional methyl group in 1A on the positive charge that forms in the process (**Table 4**, influence A) but also about an influence of the other explicit difference, i.e. carbonyl vs. alkenyl, on the positive charge (Table 4, influence B):

> *Marie: Well, if I now compare A and B… Well, because theoretically, as a resonance structure for A, this double bond could also flip up to the oxygen [draws resonance structure, Table 4, influence B]. That means, we would have a negative charge at the oxygen and a positive charge at the carbon at the carbonyl group. But then we would have two positive charges next to each other and this is, well, this is very unfavorable. That means, in this case B would be more stable than A. […]*
>
> *Interviewer: […] Why is this so unfavorable?*
>
> *Marie: Because two positive charges actually repel each other.*

Table 3. Implicit influences identified by each student in the first part of the interview without the scaffold and in the second part of the interview with the scaffold. For the initial reasoning processes without the scaffold (w/o), two details are provided (I | RS): whether a student identified a frequently[A] used influence (I) and whether the student communicated the influence in the theoretically proposed reasoning structure (RS). For the reasoning process with the scaffold (w/), it is displayed whether a student incorporated a frequently[A] used influence into the structure of the scaffold (S).

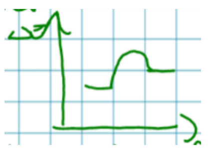
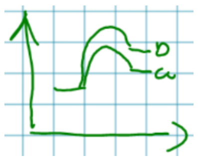
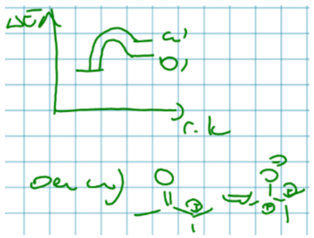
Students	Frequently[A] used implicit influences for problem 1						Frequently[A] used implicit influences for problem 2					
	e^- donation (CH_3 in 1A, plausible)		e^- delocalization (C=C in 1B, plausible)		e^- withdrawal (C=O in 1A, plausible)		e^- donation (*t*-Bu in 2A, plausible)		e^- withdrawal (Cl in 2A, implausible)		relief of B-strain (*t*-Bu in 2A, plausible)	
	w/o I | RS	w/ S	w/o I | RS	w/ S	w/o I | RS	w/ S	w/o I | RS	w/ S	w/o I | RS	w/ S	w/o I | RS	w/ S
Anna	✗	✗	✗	✗	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✗	✗
Annika	✓ | ✓	✓	✗	✗	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✗
Fabian	✓ | ✓	✓	✓ | ✓	✓	✗	✗	✓ | ✓	✓	✓ | ✓	✓	✗	✓
Felix	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✓ | ✓	✗	✗	✗
Franziska	✗	✗	✗	✗	✓ | ✓	✓	✗	✗	✗	✗	✗	✓
Isabell	✓ | ✓	✓	✗	✗	✗	✓	✓ | ✓	✓	✓ | ✓	✓	✗	✗
Jan	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✗	✓	✗	✗	✗	✗
Julia	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗	✗
Laura	✗	✗	✗	✗	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✓
Leon	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✗	✗	✗
Marcel	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✗	✗	✗	✗
Marie	✓ | ✓	✓	✗	✗	✗	✓	✓ | ✓	✓	✗	✗	✗	✗
Michelle	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✗	✗	✗	✓
Mona	✗	✓	✗	✗	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✗	✗
Niklas	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✗
Nina	✓ | ✓	✓	✓ | ✓	✓	✗	✓	✓ | ✓	✓	✗	✓	✗	✗
Philipp	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✗	✓
Sarah	✗	✗	✗	✗	✓ | ✓	✓	✗	✗	✗	✗	✗	✗
Tim	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✓ | ✓	✓	✗	✗	✗	✗
Yannick	✓ | ✓	✓	✗	✗	✓ | ✓	✓	✓ | ✓	✓	✗	✗	✗	✗

(green): Implicit influences that students identified without the scaffold, communicated in the theoretically proposed reasoning structure in this initial problem solving process, and incorporated into the structure of the scaffold

(blue): Implicit influences that students did not identify without the scaffold but identified with the scaffold

[A] We defined frequently used influences as those that were identified by more than 2 students.

Table 4. Marie's entries (in green) when using the scaffold to reason about problem 1. Her written work was translated from German into English.

	Difference 1 *atom or group of atoms difference between A and B?* A) 3 B) 2	Difference 2 *atom or group of atoms difference between A and B?* A) C=O B) C=C
Property change 1 *property change of the reactant that increases or decreases the energy of the reactant?* carbocation forms  a positive charge forms octet rule isn't fulfilled	Influence A *influence of the difference (above) on the property change (left) / effect on the change in energy?*  the +I effects stabilize the positive charge A has two substituents with +I effect and B one	Influence B *influence of the difference (above) on the property change (left) / effect on the change in energy?*  two positive charges next to each other are very unfavorable

With the scaffold, Marie identified two implicit influences. When solving problem 1 by herself, she did not identify electron withdrawal toward the carbonyl oxygen, however, with the scaffold, she explained that the electron-withdrawing effect of the oxygen leads to repulsion between nuclei carrying positive charge and supported this with a drawing (**Table 4**, influence B). This influence, which was not taught to the students in the context of carbocation formation, was identified by 6 more students with the scaffold than without the scaffold (**Table 3**). A small increase in consideration of the other plausible influences embedded in problem 1 can be seen in **Table 3**.

Table 3 also demonstrates that 4 students identified all influences that were embedded in the problem design (cf. **Table 1**) in their initial problem solving processes and 9 students did so when they were supported by the scaffold. Thus, a ceiling effect of the number of identified influences could be observed for problem 1.

Table 5. Number of implicit influences identified by each student in the first part of the interview without the scaffold (w/o) and in the second part of the interview with the scaffold (w/).

Students	Number of implicit influences identified for problem 1		Number of implicit influences identified for problem 2	
	w/o	w/	w/o	w/
Anna	1	1	1	2
Annika	2	2	1	2
Fabian	2	3	2	3
Felix	2	3	2	1
Franziska	1	1	0	2
Isabell	1	2	2	2
Jan	2	3	1	2
Julia	0	0	0	0
Laura	2	2	1	3
Leon	2	3	2	2
Marcel	3	3	1	1
Marie	1	2	2	2
Michelle	3	3	1	2
Mona	1	2	1	2
Niklas	2	3	1	2
Nina	2	3	1	2
Philipp	3	3	2	3
Sarah	1	1	0	0
Tim	3	3	1	1
Yannick	2	2	2	2

[shaded]: Problem solutions in which students considered more implicit influences with the scaffold than without the scaffold

When solving problem 2 by themselves, only Leon and Yannick reasoned about bromide being the better leaving group due to better accommodation of negative charge. Because **Table 3** only displays influences that were utilized by more than two students, the identification of this plausible influence is not shown. Instead, in their initial problem solving processes, 7 students identified the implausible influence that greater electron withdrawal toward chlorine would lead to an easier departure of chloride compared to bromide (**Table 3**). While the rationale that higher electronegativity increases leaving group ability is chemically sound, it is an implausible influence for ranking the leaving group abilities of chloride and bromide because the different sizes of the halides have a greater influence on their leaving group abilities. In a recent study conducted in the US (Popova & Bretz, 2018), OC II students also used this influence on the leaving group ability of halides more often than the plausible influence of greater charge accommodation. In our study, 3 students who had not identified this implausible influence without the scaffold identified it with the scaffold, while plausible influences were identified by 9 more students, i.e. electron donation of the tert-butyl group and relief of B-strain (**Table 3**). This demonstrates that the scaffold does not influence students to modify their reasoning toward higher plausibility but helps them to identify more implicit influences. Identifying all chemically sound implicit influences of explicit differences on changes, e.g. that greater electronegativity and larger size lead to greater leaving group ability, is an important step of multivariate mechanistic reasoning that is supported by the scaffold. In addition, our results demonstrate that the scaffold helped 5 students to identify the relief of B-strain (**Table 3**), a plausible influence that the students had not encountered in their coursework and that no student identified without the scaffold. Hence, this is an indicator that the scaffold can support transfer of knowledge.

In the following, we provide the example of Laura solving problem 2, which not only exemplarily demonstrates reasoning about electron withdrawal toward chlorine (an implausible influence) and the relief of B-strain (a plausible influence that required transfer effort) but can also be used to summarize our main findings regarding the research questions.

With respect to research question 1a, we found that, without the scaffold, students always communicated implicit influences they identified in the theoretically proposed reasoning structure on which the scaffold is based (**Table 3**). For example, Laura used electron withdrawal toward chlorine to describe an influence of the explicit difference chlorine vs. bromine on a change that occurs in every leaving group departure step, i.e. electron movement:

> *Laura: I think I have learned once, or I also think I can explain that chloride is a better leaving group than bromide because… let's see [looks into the periodic table]… it's much more electronegative. Well, not so much. But the electronegativity is a bit higher than in the case of bromide. […] Then the activation energy is smaller in A than in B. Okay.*
>
> *Interviewer: Can you explain in greater detail why the electronegativity of chlorine causes the activation energy to be lower?*
>
> *Laura: Chlorine pulls the electrons at this position more strongly and takes them along as a leaving group more easily if it's more electronegative [than bromine].*

Laura also incorporated the same influence into the structure of the scaffold. This can be seen in her entry for influence A in the table (**Table 6**) provided to her in the second part of the interview.

With respect to research question 1b, it was generally observed that students incorporated the influences they identified without the scaffold into the structure of the scaffold. Hence, our results to both subquestions of the first research question demonstrate that the structure provided by the scaffold builds on what students already do when engaging in comparative mechanistic reasoning by themselves.

Table 6. Laura's entries when using the scaffold to reason about problem 2. Her written work was translated from German into English.

	Difference 1 *atom or group of atoms difference between A and B?* reactant A: Cl^- as a leaving group reactant B: Br^- as a leaving group	Difference 2 *atom or group of atoms difference between A and B?* reactant A: 2x ethyl and 1x *tert*-butyl at 1 [carbon attached to the leaving group] reactant B: 2x ethyl and 1x methyl at 1 [carbon attached to the leaving group]
Property change 1 *property change of the reactant that increases or decreases the energy of the reactant?* formation of a carbocation → increase in energy → charge	Influence A *influence of the difference (above) on the property change (left) / effect on the change in energy?* Cl higher electronegativity than Br → stronger -I substituent → Cl^- as a better leaving group → increase in energy in A lower than in B	Influence B *influence of the difference (above) on the property change (left) / effect on the change in energy?* *tert*-butyl in A greater +I substituent → stabilizes charge better than methyl group → increase in energy in A lower than in B
Property change 2 *property change of the reactant that increases or decreases the energy of the reactant?* change in symmetry of the molecule and bond angle → larger bond angle → decrease in energy because of steric reasons	Influence C *influence of the difference (above) on the property change (left) / effect on the change in energy?*	Influence D *influence of the difference (above) on the property change (left) / effect on the change in energy?* more space for larger substituent (*tert*-butyl) matters more than more space for smaller substituent (methyl) → decrease in energy in A greater than in B

With respect to research question 2, we found that 15 students identified more implicit influences with the scaffold than without the scaffold, at least for one problem solution (**Table 5**). While for most of these students the scaffold helped them to identify one more influence (**Table 5**), Laura identified two more influences. When reasoning about the influence of the explicit difference tert-butyl vs. methyl on the formation of positive charge of the carbocation, Laura identified electron donation, which she had not identified when solving the problem by herself:

> *Laura: Now we just have the difference that one substituent in A is larger than in B, or it's a stronger +I substituent than in B. That means, I think that the carbocation in A is more stabilized than in B. And so the increase in energy in A is again lower than in B.*
>
> *Interviewer: Why is this a stronger +I substituent, or what does that mean?*
>
> *Laura: […] I learned once, the larger the substituent, the stronger the I effect, +I effect. […]*
>
> *Interviewer: What does the term stabilized mean in this sentence?*
>
> *Laura: I had said there is a +I substituent. That means the positive charge is stabilized by the electrons that are pushed toward it, yeah, stabilized, like weakened.*

Laura noted the implicit influence +I effect in the table provided during the scaffolding process (**Table 6**, influence B). Additionally, when reasoning about the relation between the explicit difference tert-butyl vs. methyl and the change in bond angle, Laura explained that, for a larger substituent, obtaining more space leads to greater decrease in energy than it does for a small substituent (influence D, **Table 6**):

> *Laura: Here we have the methyl substituent in one case, which is relatively small, and the tert-butyl substituent, which is quite large. And that means […] more space for a larger substituent has a greater effect than more space for a smaller substituent. That means the decrease in energy in A is greater than in B.*

Laura only explained that the substituents get more space and that this effect is greater for the bulkier substituent. She did not verbalize the decrease of electronic repulsion, still, her reasoning captured the basic idea of the relief of B-strain that she was not taught in her organic chemistry courses.

When Laura was asked how the scaffold helped her, she referred to the aspects that were the theoretical basis of constructing the scaffold and that are demonstrated by the results of our analysis:

> *Laura: Well, I think that I looked at the differences of the reactants previously [without the scaffold]. But the thing with the property change… I think this wasn't… Well, I did look at what changed, but so exactly? Well, I think it helped me that I looked at each, step by step. And otherwise [without the scaffold] I look at it once, and I'm a bit like… Now what do you do first?*

The scaffold built on what Laura and the other students already did when engaging in comparative mechanistic reasoning without the scaffold. In addition to that, it structured students' reasoning process in a stepwise fashion that, for 15 of 20 students, led to the identification of at least one more influence for one problem.

Another aspect of students' reasoning is that they often focused on a change visible in the product (e.g. the positive charge of the carbocation) instead of the actual process of change (e.g. formation of positive charge in the transition state). This dynamic aspect is required to make a sound claim about activation energy. Students' predominantly static approaches could be observed with and without the scaffold. The scaffold was designed to foster the multivariate aspect of students' mechanistic reasoning and not the dynamic aspect. This is why this finding is presented elsewhere as part of an in-depth analysis of the first part of the interviews (Caspari, Kranz, & Graulich, 2018), independent of the scaffold.

Statistics and limitations of the study

The increase in implicit influences students considered was explored for statistical significance using the paired-samples t-test. Compared to when they solved the problems by themselves, the students considered significantly more implicit influences with the scaffold ($p < 0.001$). This is coupled with a large effect size (Cohen's $d = 1.272$). While the increase is a systematic one, the statistics do not indicate causality. The increase could be caused by scaffolding, but it could also have been due to an exercise effect. It is possible that the increase was achieved simply because the students considered the same problems again or because the table provided during the scaffolding process made the students want to fill in information in empty cells. However, there was greatest increase in students' identification of influences unfamiliar to them in the context of carbocation formation, backing the interpretation that the theory-based structure of the scaffold supported the students. A future quantitative study in which students working with the scaffold are compared to students working without the scaffold can show whether this qualitative backing can be supported quantitatively. Additionally, research needs to be done to investigate whether the scaffolding positively affects students' multivariate comparative mechanistic reasoning when the scaffold is no longer provided to them and whether effects endure over time.

Conclusions and implications

When students in our study reasoned with the support of a scaffold about case comparisons of two molecules that differ by more than one explicit feature, they identified more than one implicit influence in 31 of 40 problem solutions. This high level of identification of more than one implicit influence is remarkable for two reasons. First, previous studies have demonstrated that the multivariate aspect is often missing in organic chemistry student reasoning (Bhattacharyya, 2006, 2014; Kraft et al., 2010). Second, Weinrich and Sevian (2017) have shown that the identification of implicit influences requires a high level of abstractness.

Further research needs to be done to investigate how to support students like those 5 students in our study for whom the scaffold alone did not support identification of more influences. In addition, we need to know how to facilitate students' progress toward the identification of plausible influences. To these ends, one approach might include a combination of case comparisons, scaffolding, and instruction about implicit influences, a notion supported in part by a meta-analytic review suggesting that a combination of case comparisons with instruction can be more effective for learning concepts than case comparisons alone (cf. Alfieri et al., 2013).

Our study has shown that the structure provided by the scaffold builds on the structure that students already use to engage in comparative mechanistic reasoning by themselves. For teaching practice, this indicates that this type of scaffolding can be smoothly integrated into existing teaching practices in order to expand upon what students already do and to help them identify more influences. The application of the scaffold is not limited to the case of a leaving group departure step, for which our study has shown promising results, because its structure is applicable when comparing two reactants in any type of mechanistic step, e.g. for the case comparisons proposed by Graulich and Schween (2018).

Furthermore, the structure of the scaffold could find applicability in other fields not tested in the exploratory study presented herein. In the following, we present one option for how the structure of the scaffold could be applied to an example used previously to investigate physics students' mechanistic reasoning (Russ, Scherr, Hammer, & Mikeska, 2008): the comparison of two falling objects. Students could be asked to compare two pieces of paper in DIN A4 format. They could be given the information that one of them has a mass of 5.0 g and is crumpled, while the other one has a mass of 7.5 g and is not crumpled. One could ask which of the two pieces of paper will reach the ground first when they are dropped from the same height? First, the students could list changes during the process that can be considered separately, e.g. that the objects experience air friction and that the objects experience gravitational acceleration (**Figure 4**, changes 1-2). Next, the students could list the differences between the two pieces of paper, i.e. mass and shape (**Figure 4**, differences 1-2). The listed differences and changes can then serve as starting and end points to infer influences of the differences on the changes (**Figure 4**, influence A-D). The students could be asked for each combination of difference and change what influence does the difference have on the change? The difference in mass influences neither the air friction nor the gravitational acceleration appreciably. The difference in shape has no influence on the gravitational acceleration. But the shape does have an influence on the air friction: The shape of the crumpled paper leads to lower air friction than the shape of the not crumpled paper. Thus, the crumpled paper reaches the ground first. In our opinion, the reasoning structure we developed based on work in philosophy of organic chemistry provides anchors for comparative mechanistic reasoning in all sciences, which needs to be confirmed in further research.

To summarize the general function of the scaffold, we want to use the words of a student in our study, Franziska, who was asked to explain which aspects of the scaffold she found helpful for solving the mechanism problems. Franziska said that the scaffold is a "guide for how to proceed. So that, through this [through the scaffold], you get points of reference on which you can then expand."

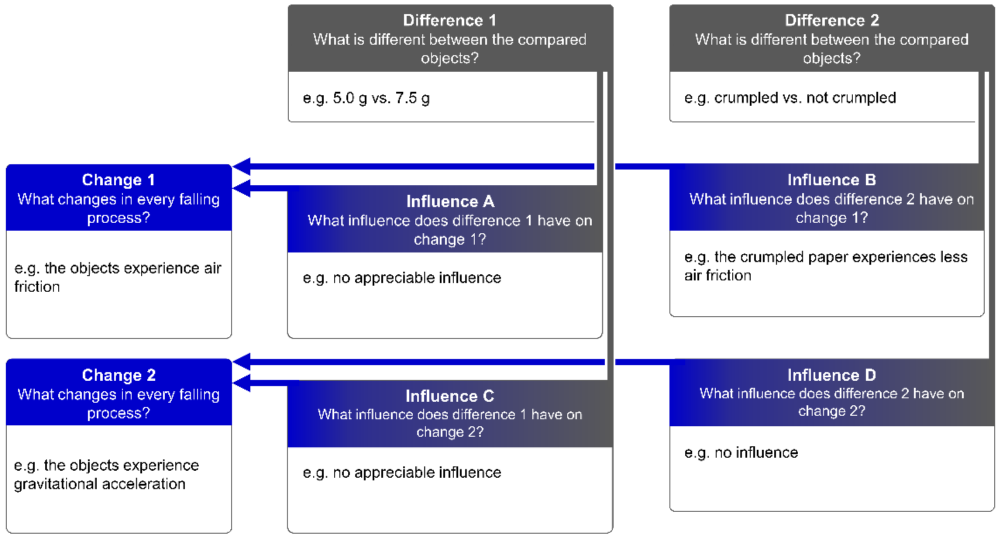


Figure 4. One option for how the structure of comparative mechanistic reasoning could be applied to a physics example to answer the question *which of two pieces of paper (first: 5.0 g and crumpled, second: 7.5 g and not crumpled) will reach the ground first when they are dropped from the same height?*

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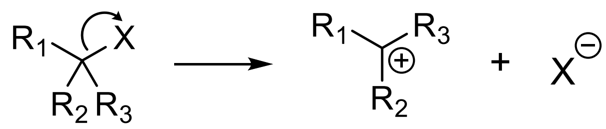
Appendix

Instructions given to the students for the scaffolding process
(translated form German into English)

1. The two reaction steps A and B can be presented in a general form as follows:



In this subtask, only look at this general form.

In the process (= on the way) from the reactant to the products the energy level of the reactant changes. This change in energy is associated with change in other properties of the reactant. Identify which property changes of the reactant increase or decrease the energy of the reactant.

2. Identify all atoms or groups of atoms that differ between the reactants of the two reactions.

3. Due to the different atoms and groups of atoms, reactants A and B have different properties. These different properties have influences on the property changes of the reactants in the process. These influences lead to different amounts of energy change for reactants A and B. Explain how the property changes are influenced and which effects this has on the comparative change in energy of reactants A and B.

4. Form a hypothesis about which reaction has lower activation energy for the represented step. Start your remarks with the information you collected in the previous subtasks. Explain how you use the information to come to a hypothesis.