Tracking Mechanistic Reasoning: From Decoding Students' and Instructors' Explanations to Developing Mechanistic Explanations for Instruction

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The results documented in this dissertation were accumulated between January 2018 and April 2022 at the Institute of Chemistry Education, Justus-Liebig-University Giessen, under the supervision of Prof. Dr. Nicole Graulich.

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“Let’s teach how we think instead of what we know.”

Vicente Talanquer and John Pollard

[Talanquer, V., & Pollard, J. (2010). Let’s teach how we think instead of what we know. *Chemistry Education Research and Practice*, *11*(2)]

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I. Abstract

In Organic Chemistry, students often struggle with mechanistic problem-solving. Instead of using implicit information to explain causal relationships, students often resort to unproductive strategies such as rote memorization or manipulation of representations. The overall goal of the EYE-OC project, in which this PhD project is embedded, is the development of instructional materials that support students in the dealing with reaction mechanisms. While many studies have focused on students' problem-solving, little is known about the construction of *instructional mechanistic explanations* and their impact on students' problem-solving.

While frameworks of Chemistry Education Research suggest how mechanistic explanations should be constructed, little is known about how to build them *effectively for learners*. In this regard, Instructional Research provides general guidance. In addition, little is known about how instructors, e.g., Organic Chemistry professors, construct mechanistic explanations. In this sense, the first study applied the construct of *framing*. The qualitative content analysis focused on how instructors construct mechanistic explanations as domain experts (*expert frame*) and how they construct them for instructional contexts (*teaching frame*). The results show differences between the mechanistic explanations between frames in terms of the elaboration and structure of causal relations (e.g., increase of problem-solving approaches in the teaching frame). The results suggest that instructors are able to adapt their explanations depending on the context, which provides guidance for the design of instructional mechanistic explanations.

[Eckhard, J., Rodemer, M., Langner, A., Bernholt, S., & Graulich, N. (2022). Let's Frame It Differently–Analysis of Instructors' Mechanistic Explanations. Chemistry Education Research and Practice, 23(1), 78-99.]

Theoretical and empirical findings from different research perspectives and the results of the first study were used to develop and implement instructional mechanistic explanations with *reasoning steps* in tutorial videos. While most of the research on tutorial videos is based on best-practices examples and user evaluation, much is to be learnt about how students process the instructional explanations in tutorial videos. To test the effectiveness of the developed videos, an intervention study with qualitative content analysis was conducted to examine whether students incorporated the *reasoning steps* into their explanations. It was found that after watching the tutorial videos, students were able to infer more implicit properties and use them in their problem-solving. It was also shown that linking structural to energetic considerations before and after watching the videos is challenging. The findings indicate implementation approaches and ways in which instructional mechanistic explanations can support students in problem-solving. Moreover, they provide a basis for further development of instructional materials.

[Eckhard, J., Rodemer, M., Bernholt, S., & Graulich, N. (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning. Journal of Chemical Education, 99(6), 2231-2244.]

Through the focus on the instruction, the findings of this dissertation extend previous research on mechanistic reasoning, which has primarily focused on students' (deficient) approaches. Furthermore, the findings of the entire EYE-OC project contribute to an evidence-based exploration of the learning effectiveness of multimedia learning resources, both in terms of visual design and design of the instructional explanation.

II. Zusammenfassung

Im Bereich der Organischen Chemie (OC) begegnen Studierende häufig Herausforderungen beim Problemlösen von mechanistischen Aufgaben. Anstelle der Nutzung impliziter Informationen zur Erklärung von Kausalzusammenhängen greifen Studierende häufig auf unproduktive Strategien wie das Auswendiglernen oder die reine Manipulation von Repräsentationen zurück. Das übergeordnete Ziel des EYE-OC-Projekts, in das dieses Promotionsvorhaben eingebettet ist, war die Entwicklung von Instruktionsmaterialien, die Studierende beim Umgang mit Reaktionsmechanismen unterstützen. Während sich in der Vergangenheit viele Studien auf das Problemlösen von Studierenden im mechanistischen Denken konzentriert haben, ist wenig darüber bekannt, wie instruktionale mechanistische Erklärungen gestaltet werden und welchen Einfluss sie auf das Problemlösen haben.

Während domänenspezifische Aspekte und fachdidaktische Frameworks begründen, wie eine mechanistische Erklärung in der Organischen Chemie aufgebaut sein sollte, ist noch wenig darüber bekannt, wie sie im Instruktionskontext effektiv für Lernende gestaltet werden kann. Die Instruktionsforschung liefert hierzu allgemeine Hinweise. Zudem ist noch wenig darüber bekannt, wie Dozierende, z. B. OC-Professor:innen, als Expert:innen der Instruktion ihre mechanistischen Erklärungen aufbauen und wie sie diese für Lehrkontexte gestalten. Vor diesem Hintergrund wurde in der ersten Studie das Konstrukt des *Framings* angewendet. Im Fokus der qualitativen Inhaltsanalyse stand zum einen, wie Dozierende als Expert:innen ihrer Domäne mechanistische Erklärungen aufbauen und wie sie diese in einem Lehrkontext gestalten. Die Ergebnisse zeigen Unterschiede zwischen mechanistischen Erklärungen in Bezug auf die Elaboration von Kausalzusammenhängen sowie deren Gestaltung zwischen den Frames (z.B. stärkere Strukturierung mit Problemlöseansätzen im Lehrkontext). Die Ergebnisse lassen den Schluss zu, dass Dozierende in der Lage sind, ihre Erklärungen kontextabhängig anzupassen, woraus sich Implikationen für die Lehre ableiten lassen und Indikatoren für die Gestaltung instruktionaler mechanistischer Erklärungen gewonnen werden können.

[Eckhard, J., Rodemer, M., Langner, A., Bernholt, S., & Graulich, N. (2022). Let's Frame It Differently–Analysis of Instructors' Mechanistic Explanations. Chemistry Education Research and Practice, 23(1), 78-99.]

In einer zweiten Studie wurden aus theoretischen und empirischen Erkenntnissen der Wissenschaftsphilosophie, der fachdidaktischen Forschung, der Kognitionspsychologie sowie den Erkenntnissen der ersten Studie didaktisch aufbereitete instruktionale mechanistische Erklärungen entwickelt und in Lernvideos implementiert. Dabei wurden *Argumentationsschritte* implementiert, die den Lösungsweg einer mechanistischen Fallvergleichsaufgabe modellieren. Während die Forschung zu Lernvideos zumeist auf Best-Practice-Beispielen sowie der Nutzung und Bewertung durch die Zielgruppe basiert, ist wenig darüber bekannt, wie Studierende die instruktionalen Erklärungen in den Lernvideos verarbeiten. Um die Wirksamkeit zu testen, wurde daher mittels qualitativer Inhaltsanalyse untersucht, ob und wie die Studierenden die *Argumentationsschritte* in ihre Erklärungen übernehmen. Es zeigt sich, dass die Studierenden nach dem Betrachten der Lernvideos in der Lage sind, mehr strukturelle Eigenschaften abzuleiten und für ihre Problemlösung zu nutzen. Es zeigt sich aber auch, dass die Verknüpfung von strukturellen Überlegungen mit dem energetischen Verlauf auch nach dem Ansehen der Videos eine Herausforderung darstellt. Die Ergebnisse zeigen Implementationsansätze auf, wie die

instruktionalen mechanistischen Erklärungen die Studierenden beim Problemlösen unterstützen können. Darüber hinaus bieten sie eine Grundlage für die Weiterentwicklung von digitalen Instruktionsmaterialien.

[Eckhard, J., Rodemer, M., Bernholt, S., & Graulich, N. (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning. Journal of Chemical Education, 99(6), 2231-2244.]

Durch die Fokussierung auf die Instruktion erweitern die Erkenntnisse dieser Dissertation die bisherige Forschung zum mechanistischen Denken, die sich vor allem auf die (defizitären) Herangehensweisen der Studierenden konzentrierte. Darüber hinaus tragen die Erkenntnisse des gesamten EYE-OC-Projekts dazu bei, die Gestaltung und Lernwirksamkeit multimedialer Lernressourcen evidenzbasiert zu ergründen, und zwar sowohl im Hinblick auf die visuelle Gestaltung als auch im Hinblick auf die Gestaltung instruktionaler Erklärungen.

III. List of Publications and Conference Proceedings

Papers in Peer-reviewed Journals

First-author Paper

- Eckhard, J., Rodemer, M., Langner, A., Bernholt, S., & Graulich, N. (2022). Let's frame it differently–analysis of instructors' mechanistic explanations. *Chemistry Education Research and Practice*, *23*(1), 78-99.

- Eckhard, J., Rodemer, M., Bernholt, S., & Graulich, N. (2022). What do university students truly learn when watching tutorial videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning. *Journal of Chemical Education*, *99*(6), 2231-2244.

Co-author Paper

- Rodemer, M., Lindner, M. A., Eckhard, J., Graulich, N., & Bernholt, S. (2022). Dynamic signals in instructional videos support students to navigate through complex representations: An eye-tracking study. *Applied Cognitive Psychology*, *36*(4), 852-863.

- Rodemer, M., Eckhard, J., Graulich, N., & Bernholt, S. (2021). Connecting explanations to representations: benefits of highlighting techniques in tutorial videos on students' learning in Organic Chemistry. *International Journal of Science Education*, *43*(17), 2707-2728.

- Rodemer, M., Eckhard, J., Graulich, N., & Bernholt, S. (2020). Decoding case comparisons in Organic Chemistry: Eye-tracking students' visual behavior. *Journal of Chemical Education*, *97*(10), 3530-3539.

Peer-Reviewed Book Chapter

- Bernholt, S., Eckhard, J., Rodemer, M., Langner, A., Asmussen, G., & Graulich, N. (2023). Designing tutorial videos to support students' learning of reaction mechanisms in Organic Chemistry. In: Y. J. Dori, C. Ngai, G. Szteinberg (eds.). *Digital Learning and Teaching in Chemistry: An International and Inclusive Approach.* Royal Society of Chemistry Publishing.

- Graulich, N., Rodemer, M., Eckhard, J., & Bernholt, S. (2022). Gibt es ideale Blickbewegungsmodelle zur Förderung der Lernenden beim Lösen organisch-chemischer Aufgaben?.(Do ideal eye-movement models exist to support learners to solve organic-chemistry tasks?). In: Klein, M. Schindler, N. Graulich, J. Kuhn (eds). *Eye-Tracking in der Mathematik-und Naturwissenschaftsdidaktik: Forschung und Praxis* (pp. 1-18). Springer Berlin Heidelberg.

- Asmussen, G., Rodemer, M., Eckhard, J., & Bernholt, S. (2022). From free association to goal-directed problem-solving—Network analysis of students' use of chemical

concepts in mechanistic reasoning (pp. 90-109). In: Graulich, N., Shultz, G. (eds). *Student Reasoning in Organic Chemistry*. Royal Society of Chemistry Publishing.

Conference Proceedings

- Eckhard, J., Rodemer, M., Bernholt, S., Graulich, N. (2021), „Welches Erklärniveau?“ - Analyse von Erklärungen von Dozierenden der Organischen Chemie, In: S. Habig (Hrsg.), *Naturwissenschaftlicher Unterricht und Lehrerbildung im Umbruch?*. Gesellschaft für Didaktik der Chemie und Physik, digitale Jahrestagung 2020, S. 216. URL: https://www.gdcp-ev.de/wp-content/tb2021/TB2021_216_Eckhard.pdf

- Eckhard, J., Rodemer, M., Bernholt, S. & Graulich, N. (2019), Blickbewegungen beim Umgang mit organischen Reaktionsmechanismen, In: C. Maurer (Hrsg.), *Naturwissenschaftliche Bildung als Grundlage für berufliche und gesellschaftliche Teilhabe, Gesellschaft für Didaktik der Chemie und Physik*. Jahrestagung in Kiel 2018, S. 807, Universität Regensburg. URL: http://www.gdcp.de/images/tb2019/TB2019_807_Eckhard.pdf

Oral Presentations

- BCCE 2022: Biennial Conference on Chemical Education 2022: Purdue/IN 31.07.-04.08.2022, Titel: *How to design tutorial videos in Organic Chemistry and what do students truly learn from them?*

- GDCP Jahrestagung 2021 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)): Unsicherheit als Element von naturwissenschaftsbezogenen Bildungsprozessen, Virtuell, 13.09.-16.09.2021, Titel: *Einfluss von OC-Lernvideos auf das mechanistische Erklären.*

- GDCP Jahrestagung 2020 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)): Naturwissenschaftlicher Unterricht und Lehrerbildung im Umbruch?, Virtuell, 14.-17.09.2020, Titel: *„Welches Erklärniveau?“ - Analyse von Begründungen von OC-Dozierenden.*

- BCCE 2020: Biennial Conference on Chemical Education 2020: Corvallis/OR, 18.-23.07.2020, Titel: *Let’s frame it differently: Analyzing mechanistic explanations of Organic Chemistry instructors*. Abstract accepted March 31, 2020. Because of the global COVID-19 pandemic, the 2020 Biennial Conference on Chemical Education was terminated on April 2, 2020, by the Executive Committee of the Division of Chemical Education, American Chemical Society; and, therefore, this presentation could not be given as intended.

- BCCE 2020: Biennial Conference on Chemical Education 2020: Corvallis/OR, 18.-23.07.2020, Titel: *Identifying decoding behavior in case comparison tasks on mechanistic problems in Organic Chemistry*. Abstract accepted March 31, 2020. Because of the global COVID-19 pandemic, the 2020 Biennial Conference on Chemical Education was terminated on April 2, 2020, by the Executive Committee of

the Division of Chemical Education, American Chemical Society; and, therefore, this presentation could not be given as intended.

- GDCP Jahrestagung 2019/FDdB im VBio 2019 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)): Naturwissenschaftliche Kompetenzen in der Gesellschaft von morgen, Wien, 09.-12.09.2019, Titel: *Dekodieren organisch-chemischer Reaktionen: Eine Eye-Tracking Studie.*

- GDCP Jahrestagung/FDdB im VBio 2019 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)), Naturwissenschaftliche Kompetenzen in der Gesellschaft von morgen, Wien, 09.-12.09.2019, Titel: *Lernen mit Hervorhebungen in Video-Tutorials in der Organischen Chemie.*

- 35. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht (Annual conference of the German Chemical Society (GDCh) - special interest group: Chemistry Education), Karlsruhe, 13.-15.09.2018, Titel: *Ins Auge gefasst: Untersuchung gruppenspezifischer Unterschiede beim Umgang mit Reaktionsmechanismen unter Verwendung von Eye-Tracking - EYE-OC.*

Poster Presentations

- Royal Society of Chemistry: #RSCPoster Twitter Conference, 2021, Titel: *How to navigate students through organic representations*, URL: https://twitter.com/JuliaEckhard/status/1366716789208604673.

- GDCh-Wissenschaftsforum Chemie 2019 (Annual conference of the German Chemical Society (GDCh)): 36. Fortbildungs- und Vortragstagung der GDCh-Fachgruppe Chemieunterricht (special interest group: Chemistry Education), Aachen, 16.-19.09.2019, Titel: *Gruppenspezifisches Dekodierverhalten beim Lösen mechanistischer Aufgaben – EYE-OC.*

- Gordon Research Conference 2019: Chemistry Education Research and Practice, Lewiston/ME, 16.-21.06.2019, Titel: *Investigation of group-specific differences when solving mechanistic problems using Eye-Tracking – EYE-OC.*

- GDCP Jahrestagung 2018 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)): Naturwissenschaftliche Bildung als Grundlage für berufliche und gesellschaftliche Teilhabe, Kiel, 17.-20.09.2018, Titel: *Blickbewegungen beim Umgang mit organischen Reaktionsmechanismen.*

Contributed Posters

- Rodemer, M., Bernholt, S., Eckhard, J., Graulich, N. (2021). *Navigating students' attention: Eye-movements in Ochem tutorials. Royal Society of Chemistry*: #RSCPoster Twitter Conference, online.

- Rodemer, M., Eckhard, J., Graulich, N., Bernholt, S. (2019). *Cueing in tutorial videos in Organic Chemistry: Investigation of learning effectiveness using Eye Tracking*. 13th

Conference of the European Science Education Research Association (ESERA), Bologna, Italy.

- Rodemer, M., Eckhard, J., Graulich, N., Bernholt, S. (2018). *Der Umgang mit Reaktionsmechanismen: Eine Eye Tracking Analyse (Dealing with reaction mechanisms: an eye tracking analysis)*. GDCP Jahrestagung 2018 (Annual conference of the German Society for Chemistry and Physics Education (GDCP)). Kiel, Germany.

- Rodemer, M., Eckhard, J., Graulich, N., Bernholt, S. (2018). *Using Eye Movement Modelling Examples as an instructional tool in Organic Chemistry*. 2018 Summer School of the European Science Education Research Association (ESERA), Jyväskylä, Finland.

1. Introduction

Today's challenges, such as climate change, resource availability, infectious diseases, and global hunger, that we face as a society – but also as individuals – are strongly linked to scientific phenomena and processes. Making sense of these requires the ability to construct theory- and evidence-driven scientific explanations (Braaten and Windschitl, 2011; Krell *et al.*, 2022). Hence, it is undeniable that the construction of scientific explanations needs to be encouraged in Science Education.

In the field of Organic Chemistry, constructing scientific explanations is considered part of the organic chemist's daily business. Organic chemists are required to make sense of phenomena and (new) reaction mechanisms, i.e., to understand, control and predict them by building mechanistic explanations. This ability is not only part of the professional expertise of chemists, but has been shown to be a predictor of student success, e.g., not only in solving unfamiliar mechanisms (Grove *et al.*, 2012), but also in passing non-major courses (Betancourt-Pérez *et al.*, 2020). Therefore, to promote students' problem-solving skills, it is important to foster the construction of well-reasoned mechanistic explanations.

An enormous number of studies have characterized students' (deficit) strategies to construct explanations in Organic Chemistry (for reviews see: Graulich, 2015; Dood and Watts, 2022), leading to the development of instructional approaches, such as interventions and curricular changes (Flynn and Ogilvie, 2015; Cooper *et al.*, 2019) and course modifications (Flynn, 2015), the implementation of explicit prompting (Crandell *et al.*, 2018), and scaffolding (Caspari and Graulich, 2019; Keiner and Graulich, 2021). However, approaches have paid little attention to mechanistic explanations *in instruction* and their effectiveness on students' construction of mechanistic explanation when solving mechanistic tasks. Thus, the guiding question of this dissertation arises:

HOW SHOULD INSTRUCTIONAL EXPLANATIONS BE DESIGNED TO SUPPORT STUDENTS' CONSTRUCTION OF MECHANISTIC EXPLANATIONS IN ORGANIC CHEMISTRY?

To answer the guiding question, the foundations of constructing instructional explanations need to be explored and related to the discipline of Organic Chemistry by synthesizing theoretical and empirical findings from multiple disciplines. Furthermore, evidence on how Organic Chemistry instructors provide explanations is needed to develop instructional explanations in order to contribute insights from practice. To further address the guiding question, evidence of how students process the developed instructional explanations is needed to draw conclusions about the effectiveness of the instructional explanations.

In the next chapter, the theoretical background for the development of instructional explanations is reviewed, followed by the research objectives for the development and testing of instructional explanations in Organic Chemistry.

2. Theoretical Background: Developing Instructional Explanations in Organic Chemistry

In order to approach the guiding question about the construction of instructional explanations in Organic Chemistry theoretically and empirically, it is broken down into sub-questions:

I. What constitutes a well-reasoned explanation in Organic Chemistry?
II. How can an instructional mechanistic explanation in Organic Chemistry be designed to be effective for learners?
III. What kind of instruction may be appropriate for providing mechanistic explanations in Organic Chemistry?

First, theoretical considerations from Philosophy of Science, Philosophy of Organic Chemistry and empirical results from Chemistry Education Research are discussed in order to identify the basis for (I) what constitutes well-reasoned explanations *in Organic Chemistry*. Second, considerations and findings from Instructional Research and Multimedia Research in combination with findings from Chemistry Education Research are used to explore (II) how an instructional explanation can be designed to be *effective for learners*, i.e., which considerations increase the likelihood of an instructional explanation being understood by learners. Third, it is explored (III) what kind of instruction may be appropriate for providing instructional mechanistic explanations regarding evidence-based assumptions from Instructional Research, Cognitive Psychology Research, and Multimedia Research.

(I) What Constitutes a Well-Reasoned Explanation in Organic Chemistry?

In order to identify what constitutes a well-reasoned explanation in Organic Chemistry, the first step is to look at the nature of the questions proposed in Organic Chemistry that need to be explained. To examine the construction of an explanation of these questions, it will be shown which *aspects* are envisaged by Philosophy of Science to answer such questions. Subsequently, frameworks of Chemistry Education Research will be presented to clarify how aspects are envisaged to be interrelated for problem-solving in Chemistry

Education. To conclude, *key elements* that inform the construction of well-reasoned mechanistic explanations in Organic Chemistry are identified.

2.1.1. Perspective from Philosophy of Science

As the domain of Organic Chemistry regards changes organic molecules undergo, explanations are ought to answer questions that Goodwin (2003) characterized as questions regarding transformations, e.g., "*why does [reactions of type A occur faster than reactions of type B] (rather than the other way around)?*" (Goodwin, 2003, p.142). According to Philosophy of Science, questions regarding transformations, i.e., scientific explanations of phenomena, call for a *mechanistic* type of explanation. Mechanistic explanations provide accounts of conditions and processes by considering physical-chemical and materialistic-energetic principles (Dijksterhuis, 1956). Such explanations hold the view that phenomena are explained by looking at the underlying mechanisms generating the phenomena at different levels. Machamer *et al.'s* (2000) description of a mechanism concretized important *aspects* that must be present in a mechanistic explanation: *"Mechanisms are composed of both entities (with their properties) and activities. Activities are the producers of change. Entities are the things that engage in activities. Activities usually require that entities have specific types of properties. […] The organization of these entities and activities determines the ways in which they produce the phenomenon. Entities often must be appropriately located, structured, and oriented, and the activities in which they engage must have a temporal order, rate, and duration." (Machamer et al., 2000, p. 3).* Accordingly, to construct a mechanistic explanation in Organic Chemistry, the underlying *aspects*, i.e., *entities* with their *properties* with their *organization* and their *interactions*, i.e., their activities, need to be considered in order to characterize changes in mechanism, i.e., answer questions about transformations (Machamer *et al.*, 2000).

In Organic Chemistry *entities* are, for example, molecules, components of molecules such as functional groups, atoms, and electrons. *Activities* are represented by the movement of entities leading to the formation or breaking of bonds (changes in a mechanistic step). In reaction mechanisms *entities* and *activities* are represented by structural formulas and electron pushing arrows. These discipline-specific forms and tools are recognized as the internationally used "language" of the domain. In Organic Chemistry, hence, a few lines, letters and arrows represent a great deal of information (Kozma *et al.*, 2000): such as the reacting entities (e.g., acetylic salicylic acid, Figure 1), their composition (e.g., acid group, highlighted in orange in Figure 2) and (implicitly) chemical and physical *properties* (e.g., partial charges/bond dipole moments due to electronegativity of atoms/atom groups, highlighted in pink).

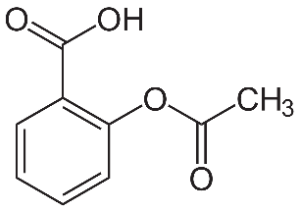

Figure 1: Structural formula of acetylsalicylic acid.

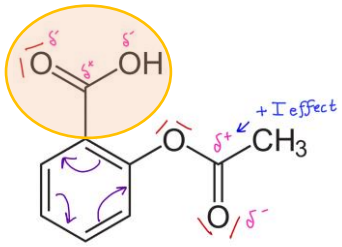

Figure 2: Structural formula of acetylsalicylic acid with some implicit information, e.g., bond dipole moments in pink.

The *aspects* suggested by Philosophy of Science that must be included in a mechanistic explanation form the basis for the construction of a well-reasoned explanation in Organic Chemistry. Considerations of Philosophy of Science have further informed the development of frameworks to characterize mechanistic reasoning and the construction of mechanistic explanations in chemistry.

2.1.2. Perspective from Chemistry Education Research

In the recent decades, several authors described reasoning frameworks to characterize students' explanations (Kraft *et al.*, 2010; Sevian and Talanquer, 2014; Becker *et al.*, 2016; Cooper *et al.*, 2016; Weinrich and Talanquer, 2016; Caspari *et al.*, 2018; Dood *et al.*, 2020). To portray reasoning, these frameworks include considerations of Philosophy of Science (i.e., proposed *aspects* and the structure of mechanistic explanations (Machamer *et al.*, 2000; Darden, 2002)) and previous educational approaches (that characterized quality and/or levels of complexity) (Brown *et al.*, 2010; Bernholt and Parchmann, 2011).

In the proposed frameworks in Chemistry Education literature[1] (Kraft *et al.*, 2010; Sevian and Talanquer, 2014; Becker *et al.*, 2016; Cooper *et al.*, 2016; Weinrich and Talanquer, 2016; Caspari *et al.*, 2018; Dood *et al.*, 2020) commonalities are evident in the categorization of reasoning approaches along a *continuum of causality*. Recent

[1] In the following referred to as „recent frameworks".

frameworks place explanations of low complexity, considering the "*what*", at the beginning of their causal continuum. These accounts tend to be descriptive (e.g., focusing on entities such as salient features of the structural formula), teleological (e.g., describing entities as acting for a particular purpose), or anthropomorphic (e.g., describing entities as acting like humans). The end of the continuum consists of explanations as some answer to the triplet of "*what*", "*how*", and "*why*" (Cooper *et al.*, 2016). For example, describing (multiple) causal factors and causal chains (Sevian and Talanquer, 2014), or by thoroughly describing causes and their effects on the change occurring during a reaction, e.g., by considering explicit and implicit factors (Caspari *et al.*, 2018). Given the importance of causality in the various frameworks, it emerges that building cause-effect relationships by identifying *causes* and *effects* is one of the most important key elements in constructing mechanistic explanations in Organic Chemistry.

In their categorizations, recent frameworks show an increase in the (complexity of) causality of mechanistic explanations. However, they place different emphasis on the analysis of explanations, which further informs the construction of well-reasoned explanations in Organic Chemistry. These differences are shown in the exemplary comparison of the frameworks of Sevian and Talanquer (2014), Cooper and colleagues (2016), and Caspari and colleagues (2018) (see Table 1). Comparing their focus of analysis, highlights aspects of an explanation for problem-solving in chemistry and how these aspects should be related in a well-reasoned mechanistic explanation.

Table 1: Summary of reasoning types of three recent reasoning frameworks to characterize mechanistic reasoning in chemistry.

Reasoning framework of Sevian and Talanquer (2014) "modes of reasoning framework"	
Modes of reasoning	**Description**
Descriptive	(Re)describing phenomena, focus on explicit salient features, without referring to a cause
Relational	Explicit and implicit features are recognized, differentiation of number of relations (uni- vs. multirelational)
Linear-causal	Influence of many factors (explicit/implicit properties) are recognized, cause-effect-relationships are discussed for single agent, linear chains in explanations (uni- vs. multirelational)
Multi-component	Static and dynamic interplay of many factors and interactions of multiple variables are considered, using explicit and implicit features to establish cause-effect-relationships, weighing of variables (isolated, vs. integrated in interconnected causal stories)

Increase in complexity of reasoning

Reasoning framework of Caspari, Kranz and Graulich (2018) "comparative mechanistic reasoning framework "	
Levels of complexity of relations	**Description**
Low complexity	Explicit structural differences/or non-electronic effect are used as a cause to describe relation to change.
Middle complexity	Explicit structural difference is used to infer implicit structural cause, which is used to describe relation to/or non-electronic effect on/change.
High complexity	Explicit structural difference is used to infer implicit structural cause, which is used to describe electronic effect on change.

Increase in complexity of relations

Reasoning framework of Cooper and colleagues "causal-mechanistic reasoning-framework" (Cooper, Kouyoumdjian, Underwood (2016), Becker, Noyes and Cooper (2016), Crandell, Kouyoumdjian, Underwood and Cooper (2018))	
	Description
Descriptive (what)	Description of what happens to the reactants and products (entities), without an indication of *how* and *why* the reaction happens
Mechanistic (what and how)	Identification of electrons as entities, explanation of their activities that lead to change of the reaction, i.e., how the reaction occurred, understanding of electron movement
Causal (what and why)	Discussion of intermolecular electrostatic attraction between entities (interaction)
Causal mechanistic (what, how, and why)	Combination of causal and mechanistic account of the reaction (e.g., attraction between entities and electron movement causing the change of the reaction)

Increase in completeness and sophistication

Sevian and Talanquer (2014) (and, as applied and adapted by (Weinrich and Talanquer, 2016; Bodé *et al.*, 2019) propose to analyze explanations in terms of the complexity, for example, differentiating between how many explicit and implicit factors, i.e., aspects, are recognized and/or if participants explain their interaction and interplay (dynamically or statically). The categorization also highlights the analysis of weighing multiple variables.

The framework of Caspari and colleagues (2018) focuses on how students explain the changes that entities undergo during an activity, i.e., a mechanistic step such as the departure of a leaving group. In doing so, the authors added to the aforementioned framework by considering the levels of complexity of the *relations* that students aim to construct between the change during the reaction step and the explicit differences of the entities, e.g., by using implicit properties to describe an effect on the change in a reaction mechanism.

Cooper and colleagues (2016, 2018) focus on the completeness and sophistication of explanations. A complete explanation is considered a *causal-mechanistic* explanation that answers the "*what*"*,* "*how*"*,* and "*why*"*.* Thus, their framework makes a clear distinction between explanations that are purely causal and those that are purely mechanistic. *Causal* explanations answer "*what*" and "*why*" by discussing intermolecular electrostatic attractions between entities (e.g., attraction of transient charges such as London dispersion forces), whereas mechanistic explanations identify the source of this interaction on entities, one scalar level below the targeted phenomenon (e.g., identification of electron movement as the source of partial charges), i.e., the *"what"* and "*how"* (Crandell *et al.*, 2018; Krist *et al.*, 2019).

When comparing the characterization of explanations in the frameworks (Table 1), for explanations to be considered causal, they require different depth of explanations through considering scalar levels (Cooper *et al.*, 2016; Crandell *et al.*, 2018), grain sizes (Caspari *et al.*, 2018) or granularities (Sevian and Talanquer, 2014; Bodé *et al.*, 2019). In the *modes of reasoning framework* (Sevian and Talanquer, 2014; Bodé *et al.*, 2019), a cause-effect relationship at different granularities is considered causal, whereas the *comparative mechanistic reasoning framework* (Caspari *et al.*, 2018) asks for causes and effects to be verbalized at an electronic level. The *causal-mechanistic reasoning framework* (Cooper *et al.*, 2016; Crandell *et al.*, 2018) requires causal explanations to be explained at a scalar level below the phenomena.

Through the comparison it is further shown that the frameworks consider different criteria e.g., linear or complex cause-effect relations of (multiple) factors (Sevian and Talanquer, 2014), or reasoning structure of students' relations (Caspari *et al.*, 2018), and dimensions

e.g., complexity and sophistication (Sevian and Talanquer, 2014; Cooper *et al.*, 2016), or complexity of relations (Caspari *et al.*, 2018) present in an explanation.

The frameworks provide guidance on what constitutes a well-reasoned mechanistic explanation, leading to the identification of *key elements*. Common to these well-reasoned mechanistic explanations is that they get to the root of the "*why*" question by combining and interrelating different aspects along the way that drive causality, respectively the complexity.

As identified through consideration of *aspects* of Philosophy of Science (Machamer *et al.*, 2000; Craver and Darden, 2013) and analysis of recent frameworks of Chemistry Education Research (e.g., Sevian and Talanquer, 2014; Becker *et al.*, 2016; Cooper *et al.*, 2016; Caspari *et al.*, 2018), *key elements* that constitute a well-reasoned mechanistic explanation in chemistry can be concluded:

- causes and effects / cause-effect-relations
    - using explicit structural features of the entities to infer implicit properties that affect the activities of the entities
- process-oriented verbalizations
    - verbalization of the activities of the entities, by verbalizing the influence of implicit properties on the processes (effect), i.e., dynamic approaches to changes in a mechanistic step
- multiple variables
    - identification and weighing of the entities, their properties and their interplay to reason about multivariate interdependencies

(II) How Can an Instructional Mechanistic Explanation in Organic Chemistry Be Designed to Be Effective for Learners?

While a scientific mechanistic explanation has the intention to provide theoretical and evidence driven accounts of how and why phenomena come about, i.e., provide logical connections (Hempel and Oppenheim, 1948), instructional explanations focus on communicating domain-specific content and concepts that lead to *understanding by the learners* (Braaten and Windschitl, 2011; Kulgemeyer, 2019). Since the previous chapter laid the foundation for *what* constitutes a mechanistic explanation, in terms of *key elements* and the providence of logical connections in mechanistic explanations, the focus now turns to the instructional perspective and *how* an instructional explanation should be designed to be *effective for learners*. Based on reviews of psychology studies on the effectiveness of instructional explanations in Educational Science (Wittwer and Renkl, 2008;

Kulgemeyer, 2019) it is suggested that the likelihood of instructional explanations being understood by learners increases when the instructional explanations…

1. are adapted to the target group's prerequisites,
2. avoid digressions and focus on important concepts and principles,
3. are integrated into learners' ongoing cognitive capacities, and
4. support active knowledge construction.

In the following, these suggestions will be specifically related to the exploration of how an instructional mechanistic explanation *in Organic Chemistry* should be designed in order to be effective.

As a first step in the sense of a didactic reconstruction, a diagnosis of the learning potential of the target group is necessary in addition to the subject-specific clarification (Gropengießer *et al.*, 2016). In order to promote the effectiveness of instructional explanations in Organic Chemistry, it is necessary to examine the explanatory approaches of chemistry students (Chapter 2.1.3). Second, criteria from "*minimal explanations*" (Carroll *et al.*, 1987; Van der Meij, 1995) are transferred to the context of reaction mechanisms to conclude on how to avoid digressions and focus on important concepts and principles (Chapter 2.1.4). Then, it is examined how instructional explanations can be integrated into cognitive activities and support students' active knowledge construction in Organic Chemistry instruction with respect to students' prerequisites (Chapter 2.1.5). The concrete instructional mechanistic explanations and their implementation can be found in Chapters 5.3 and 9.

2.1.3. Prerequisites of the Target Group: Students' Approaches

In the past, a large body of research has examined students' problem-solving and construction of explanations in Organic Chemistry (for reviews see: Graulich, 2015; Dood and Watts, 2022), which can serve as prerequisites for the construction of instructional explanations. It turns out that constructing a (well-grounded) mechanistic explanation with *aspects* and *key elements* as envisaged by Philosophy of Science and recent frameworks characterizing mechanistic reasoning in chemistry (Chapters 2.1.1, 2.1.2), is challenging for students. Several studies (e.g., Bhattacharyya and Bodner, 2005; Strickland *et al.*, 2010; DeFever *et al.*, 2015; Anzovino and Bretz, 2016) have shown that students often struggle to infer what is implicitly encoded in the structural formulas, as evidence in their reasoning. Instead, students often rely on salient entities, i.e., explicit features, rather than identifying what is implicitly encoded, e.g., describe the presence of a functional group, e.g., a methyl group (Figure 2), without inferring its properties *(+I*-effect/electron donation along a *σ*-bond) or influence on a transformation a molecule might undergo during a

reaction. A central reason for students experiencing difficulties in Organic Chemistry is related to the (missing) link between the representations, i.e., the structural formulas, and the implicit information encoded, i.e., domain-relevant information like the chemical concepts (Treagust *et al.*, 2003; Ainsworth, 2006; Graulich, 2015). On the basis of explicit features, students use strategies such as the use of simplified pattern recognition, memorization, and unproductive heuristics (Maeyer and Talanquer, 2013; Graulich and Bhattacharyya, 2017; Galloway *et al.*, 2019). For example, Weinrich's and Talanquer's (2016) study found that when students compared reaction processes, they only named salient features, such as atom names, and made claims based on familiarity with the representations (Weinrich and Talanquer, 2016). Ideally, an instructional explanation in Organic Chemistry, thus, supports students in inferring structural properties of explicit representations.

Further, it appears that students have difficulty establishing cause-effect relations with implicit information. This is found when students reason about energy in reaction mechanisms. As the discipline of Organic Chemistry often requires reasoning about transformations, e.g., reasoning why certain reactants lead to a certain outcome and follow a certain pathway (Goodwin, 2003) (Chapter 2.1.1), cause-effect-relations between structural considerations and energetic consideration are required. Research on students relating structural accounts to energetic accounts revealed challenges, e.g., in relating structural properties to changes in potential energy (Becker *et al.*, 2015) or in connecting implicit properties, respectively, structural claims to activation energy (Caspari *et al.*, 2018). A study by Macrie-Shuck and Talanquer (2020) revealed that when reasoning about the transformation of energy in bond formation processes, that of 82,8 % of their participants "[…] *many of them did not seem to fully understand the mechanism for this process and expressed incomplete or alternative views of energy transformation* […]" (Macrie-Shuck and Talanquer, 2020, p. 4230), which could be explained by considering cause-effect relations between structural changes and energetic changes in a reaction mechanism. Again, these findings indicate students struggling in building cause-effect-relations using implicit information, e.g., by considering how implicit properties affect energy-lowering of a transition state. Hence, an instructional explanation should address how to link structural considerations to changes in a reaction with regard to the energetics of a reaction.

Another prominent finding in students' problem-solving strategies is their focus on entities, and thereby neglecting considerations of the dynamic processes that lead to a change in a reaction. Research indicates that students often focused on "*representational and structural issues rather than on the more process-oriented aspects of a problem*" (Christian

and Talanquer, 2012, p. 293). Accordingly, students often show a static approach of explanations, neglecting the dynamic process entities undergo, and when treating "*inscriptions as representations of static entities, the participants rarely, if ever, explicitly spoke of the movement of electrons*" (Strickland *et al.*, 2010), hence, tend to disregard the activity of electron movements. Bhattacharyya and Bodner (2005) described that when explaining mechanisms, students often reason in a static, product-oriented manner by manipulating structural formulas and electron-pushing arrows to get to the desired product. Other studies showed that students were able to reproduce electron arrows from memorization (Grove and Lowery Bretz, 2012; Wilson and Varma-Nelson, 2018). In doing so, the student used the electron-pushing arrows only as a vehicle, without understanding the physical meaning and the chemical concept of the movement of the electrons represented by them. Further studies showed that students were able to predict products even without using the electron-pushing mechanism (Grove and Lowery Bretz, 2012; Houchlei *et al.*, 2021). With these results, it is again shown that the implicit meaning of the representation of the electron-pushing arrow is often not clear to the students. This is an obstacle to understanding the implicit processes, i.e., the movement of electrons in reaction mechanisms, and using them to construct a mechanistic explanation (Bhattacharyya, 2013). This accounts for students' recourse to more entity/product-oriented approaches instead of process-oriented approaches. Instructional explanations in Organic Chemistry should therefore support the decoding of entities, i.e., representations (explicit→ implicit), and refer to the influence of structural properties with respect to the electronic level, i.e., the movement of electrons in order to support students' process-oriented reasoning.

Students' approaches to using multiple variables and reasoning about multivariate interdependencies revealed that they had difficulty weighing and using different variables and, therefore, had difficulty engaging in multivariate reasoning to support their claims (Kraft *et al.*, 2010). Maeyer and Talanquer (2013) further identified *one-reason-decision making* as a heuristic as they identified students ranking decisions based on the comparison of a single variable (e.g., number of educts) (Maeyer and Talanquer, 2013). A study by Watts and colleagues (2021) also found that students focused only on a single part of the reaction mechanism, such as an electrophile or a nucleophile as reactants, and neglected the displayed products while discussing reactivity and thereby only activated few cognitive resources. Another study by Bhattacharyya (2014) showed that when students discussed the reactive side of multifunctional molecules, they tended to focus on a "*single parameter"* (e.g., a single functional group) when discussing multifunctional molecules (Bhattacharyya, 2014, p. 595). The strategy of focusing on one or few variables

lowers cognitive load and, hence, can be explained by the cognitive load requirements, which are very high when solving complex problems such as explaining questions regarding transformations. However, part of the organic chemist's skill set when constructing well-reasoned mechanistic explanations is to consider different reaction pathways and consider alternatives (Lieber and Graulich, 2020). This requires reasoning that takes into account multiple variables, such as the reaction conditions, each reactant, and the composition of the various reactants, i.e., their functional groups. To meet students' challenges, an instructional explanation should include support for weighing multiple variables.

Empirical findings from Chemistry Education Research show that students' approaches often do not lead to successful explanations or problem-solving in Organic Chemistry (e.g., by using strategies relying on explicit features of a representation, using unproductive heuristics or unconsciously by reducing cognitive load by focusing few variables). These findings serve for the development of instructional explanations in terms of the consideration of the needs of the target group with the aim of promoting the effectiveness of instructional explanations for learners.

2.1.4. Concise Instructional Explanations

Instructional Research suggests that in order for explanations to be effective for learners, they should be concise, provide only the information that is essential, and avoid digressions (Kulgemeyer, 2019). This concept aligns with providing "*minimal explanations"* (Carroll *et al.*, 1987; Van der Meij, 1995), which take learners' limited cognitive resources into account (Chapter 2.1.5, 2.1.6, *redundancy principle*). The purpose of these explanations is to support learning by focusing only on the relevant information that is needed to understand the topic, while also providing a logical and coherent structure (Renkl, 2002; Kulgemeyer, 2019).

In terms of coherence, and comprehensibility in accordance with students' prerequisites (cf. Chapter 2.1.3.) and in accordance with explanations in common Organic Chemistry textbooks (Vollhardt and Schore, 2011; Clayden *et al.*, 2012; Bruice, 2014), a *concise instructional explanation* of a nucleophilic substitution reaction mechanism, for example, might include the following explanatory elements: a description of the type of reaction with the description and role of the reactants, the transition state, and the products. Thereby, in terms of *conciseness,* only properties relevant to the problem, such as the properties of the nucleophile (capacity to donate electrons) or the leaving group (capacity to accumulate electrons/negative charge), should be mentioned, rather than inferring redundant information (e.g., physical properties). Further, a concise overview of the reaction

mechanism with cause-effect relations for bond formation between the nucleophile and bond breaking between the carbon center and the leaving group could foster coherence and process-orientation (Chapter 2.1.6). To further promote comprehension, reaction conditions, stereochemistry, and common examples to illustrate concepts could be referenced in the instructional explanation depending on the task prompt.

There is still little research on the explanatory elements that Organic Chemistry instructors use to promote student problem-solving. These findings would further inform the construction of instructional explanations for mechanistic explanations, along with the aforementioned assumptions about concise explanations from Instructional Research and reviewing Organic Chemistry textbooks.

2.1.5. Cognitive Processing to Foster Knowledge Construction

Educational researchers who emphasize a constructivist perspective suggest that to be effective, instructional explanations must be integrated with learners' ongoing cognitive processing to support knowledge construction (Brame, 2016; Kulgemeyer, 2018). Thus, designing and implementing instructional explanations must consider students' cognitive capacity, i.e. cognitive load.

According to Sweller's (1988) Cognitive Load Theory (CLT) and Mayer's (2005) Cognitive Theory of Multimedia Learning (CTML), learning, i.e., knowledge construction is influenced by human cognitive architecture (Sweller, 1988; Mayer, 2005; Brame, 2016). The CTML, which builds on the CLT, states that learning requires the cognitive processes of *selecting, organizing*, and *integrating* of new and old information within different memory systems (Mayer, 2021) (see also Chapter 2.1.6). According to Mayer (2021), the *sensory memory* first selects information through sensory channels by paying attention. The selected information is then transferred to the *working memory*. In the working memory, mental models (verbal and pictorial) are created and integrated with prior information from the *long-term memory* (Mayer, 2021). New information is then "stored" in the *long-term memory*. Thus, new information, must pass through the *working memory*, which has limited cognitive capacity, in order to be stored in *long-term memory,* which has unlimited cognitive capacity (Fiorella and Mayer, 2018). Hence, knowledge construction and one's cognitive capability of processing (new) information is limited by the capacity of one's working memory.

In Organic Chemistry, for example, one way of ensuring the integration of new information of the instructional explanation into the learner's cognitive processing is to address the learner's prior knowledge. The goal is to integrate new information with known information, e.g., to extend known conceptions of chemical concepts (as described in Chapter 2.1.3).

To support cognitive processing, support such as prompting, specific structuring (Seidel *et al.*, 2013), and follow-up tasks have been found to be beneficial (Kulgemeyer, 2019). For example, when dealing with reaction mechanisms, cognitive processing could be supported by providing structured prompts to key elements (entity-property/cause-effect-relationships) and concepts (e.g., nucleophilicity). In addition, different sequences of (new/known) examples and (new/known) general rules (Renkl, 2014) could be provided (see Chapter 2.1.6, *segmenting*). However, when attempting to promote cognitive processing, to reduce cognitive load, attention should also be paid to the conciseness of the instructional explanation (see Chapter 2.1.6, *redundancy principle*).

Again, findings on how Organic Chemistry instructors deliver instructional explanations (using their pedagogical content knowledge (Shulman, 1986)) add ways to support knowledge construction that can be used for the construction of instructional mechanistic explanations in Organic Chemistry. The following section examines how instructional explanations might be perceived and integrated into learners' cognitive processing by the format chosen to deliver the instructional explanation and by the design principles used.

(III) What Kind of Instruction May Be Appropriate for Delivering Instructional Mechanistic Explanations in Organic Chemistry?

The previous chapters focused on exploring what constitutes a well-reasoned mechanistic explanation (e.g., including cause-effect-relations, process-oriented verbalizations and integration of multiple variables) for Organic Chemistry and identified factors that impact the effectiveness of instructional mechanistic explanation for learners (e.g., adapting to students' prerequisites and cognitive processing). In addition, considerations from Instructional Research, Cognitive Psychology Research, and Multimedia Research provide evidence-based assumptions about the delivery of instructional mechanistic explanations that focus on adapting to students' cognitive processing.

One of the most researched findings in Chemistry Education literature about students' prerequisites is their challenge in dealing with representations, i.e., structural formulas, due to their (missing) link between the representations and the implicit information (e.g., structural properties) encoded in them (for a review see: Graulich, 2015). Therefore, the dual coding channel theory (Paivio, 1990) can be considered. This theory explains cognitive processes as operating on independent, modality-specific verbal and nonverbal (visual) channels. Thus, when visual representations are combined with verbal instructional mechanistic explanations, for example, in tutorial videos, it can be expected to facilitate students' problem-solving when dealing with reaction mechanisms (Schnotz

and Lowe, 2003; Brame, 2016; Rau, 2017). Tutorial videos and video instruction "*adds auditory engagement to visual, language comprehension and cognitive processes, and allows for more varied emphasis of the importance of content*" (Stockwell *et al.*, 2015, p.933). Tutorial videos can be regarded not only as a highly effective educational tool for visualizing complex representation and processes found in reaction mechanisms, but they also provide opportunities for implementing instructional explanations with regard to students' prerequisites and cognitive capacities to support learning. However, the fact that a tutorial video was "consumed" does not automatically mean that it appeared meaningful to a student or resulted in understanding. The consumption without further implementation in instruction might even create an illusion of having acquired knowledge (Kardas and O'Brien, 2018; Mayer, 2021; Kulgemeyer *et al.*, 2022). Hence, in order to support accessibility and increase the likelihood of student comprehension, Cognitive Psychology Research and Multimedia Research suggest that instructional videos should be designed according to instructional design principles, which are described in the following.

2.1.6. Instructional Design Principles

To explore how instructional mechanistic explanations can be meaningfully implemented in the multimedia format of video, theories of cognitive load and design principles are drawn upon, and it is shown how these principles are applied to the design of tutorial videos in Organic Chemistry.

Following CLT and CTML, the design of effective tutorial videos, includes optimizing the cognitive processing to support knowledge construction (Mayer, 2005). Within this regard Mayer (2021) stated that "*the challenge for instructional designers is to effectively use the learner's visual and verbal channels to allow for active cognitive processing while not overwhelming the learner's processing capacity"* (Mayer, 2021, p. 2). Therefore, evidence-based principles for the design of tutorial videos based on CTML were proposed (Mayer, 2021). These principles regard *reducing extraneous processing* (Mayer, 2021), i.e., reducing extraneous load that does not serve learning. The five principles are: *coherence, signaling, redundancy, spatial,* and *temporal continuity*. These principles ought to guide learners' attention to the relevant content, e.g., by using visual cues (*signaling principle*) or reduction of irrelevant or distracting aspects (*redundancy principle*), which is also in line with reducing the cognitive load by attempting to provide concise explanations (Chapter 2.1.4). Pertaining to designing tutorial videos for problem-solving in Organic Chemistry, the combination of concise verbal instructional mechanistic explanations with visual highlights could direct students' attention to relevant parts of the entities referred to (Ozcelik *et al.*, 2010; van Gog, 2014). This approach also aims at increasing coherence.

Further principles aim to support the *management of essential processing* (Mayer, 2021) by reducing the intrinsic load of the content. This can be achieved through structuring or chunking the content (*segmenting*), e.g., by implementing structuring prompts or reasoning steps for solving reaction mechanisms, including an instructor's voice instead of words (*modality*) or reduction in cognitive load due to prior introduction of specific names or concepts (*pre-training*).

Mayer (2021) further introduces principles that *foster generative processing* (Mayer, 2021), i.e., enhance germane load, that is needed to meet the learning objective and supports learners' motivation and engagement, e.g., through using an appealing human voice, conversational language (*personalization)* or implementing generative learning activities like using interactive questions to improve memory and knowledge-construction (Fiorella and Mayer, 2018; Mayer, 2021). These design principles (e.g., *coherence, redundancy, segmenting*) along with considerations of which key elements to implement and how to construct effective instructional explanations for learners, inform how instructional mechanistic explanations can be constructed and implemented in tutorial videos to support problem-solving in Organic Chemistry.

2.1.7. Choosing a Task Format to Support Students' Active Learning in Instruction

To support students' active learning and engagement in instruction, a task format needs to be chosen with regard to the learners' cognitive processing (Brame, 2016; Mayer, 2021). Traditional tasks in instruction and assessment in Organic Chemistry often ask students to *predict the product* of specific reaction mechanisms (Stowe *et al.*, 2021). In these instructions "*what*" questions are often asked, such as "*what are the products for reaction XY*?", which tempt students to memorize mechanisms or simply manipulate structural formulas (Stowe and Cooper, 2019). As a result, students are often not asked to reason and explain in depth, nor are they asked (or the task does not require) to use conceptual understanding. Consequently, students are often not actively engaged, which in turn leads to a decrease in active knowledge construction (Stowe *et al.*, 2021; DeGlopper *et al.*, 2022). Therefore, with respect to the latter, a task format is needed that promotes students' active engagement. An appropriate task format is a case comparison task (see Figure 6). Case comparison tasks have been shown to actively engage individuals in problem-solving and promote deeper reasoning through comparing and weighing variables (Alfieri *et al.*, 2013).

In the context of Organic Chemistry, case comparison tasks have also been developed by Schween and Graulich (2018). In these tasks, two comparable reactions need to be contrasted, for example with regard to relative speed of each reaction step (for examples,

see tasks solutions of study 1, Appendix 10.3, p. 123). To this end, one must consider which of the two reactions has a lower activation energy in order to decide which reaction/reaction step is faster. This depends on the potential energy of the transition states. By inferring information from the structural formulas of each reaction, such conclusions about the transition states can be made (Goodwin, 2003). In doing so, one needs to "*[…] form a bridge between structure and energy*" (Goodwin, 2003, p. 144), i.e., structural and energetic accounts must be connected (Goodwin, 2003; Goodwin, 2007; Caspari *et al.*, 2018). In order to do so, individuals need to draw inferences about the similarities and differences between the cases by looking at the explicit structural differences. Further, implicit properties and concepts need to be inferred and weighed in terms of their influence on the course of the reaction (Caspari *et al.*, 2018). Thus, an explanation of a case comparison can be expected to include several relations, i.e., structural causes and resulting effects on structural changes during the reaction within the structural account. The structural account further relates to the energetic account (Goodwin, 2003), by inferring considerations about the transition state (→HAMMOND postulate, BELL-EVANS-Polanyi principle) (Goodwin, 2003; Bruice, 2014; Schmitt and Schween, 2020). Comparing, inferring and weighing structural properties challenges students' active engagement and, thus, is ought to support students' active learning. This claim is supported by the findings of studies using case comparisons in Organic Chemistry, as it is shown to be a useful tool for eliciting reasoning (Bodé *et al.*, 2019; Watts *et al.*, 2021) and fostering mechanistic reasoning (Graulich and Bhattacharyya, 2017; Caspari and Graulich, 2019; Kranz *et al.*, 2023).

Thus, through discussing and identifying

(I) what a well-reasoned explanation in Organic Chemistry includes (e.g., reasoning about entities and properties (aspects), building cause-effect relations (*key elements*), and

(II) how an instructional explanation in Organic Chemistry can be designed to increase effectiveness for learners (e.g., adaptation to chemistry students' prerequisites in explanatory approaches), and

(III) what instructional format with design principles and task format may be appropriate for instruction (e.g., redundancy principle in tutorial videos, case comparison tasks),

it was shown how an effective instructional explanation in Organic Chemistry could be constructed and implemented in instruction.

In the following, the research objectives (Chapter 3) and the studies conducted (Chapter 4) are presented to further outline the intentions to extend the findings reviewed in Chapter 2. This is followed by the results and discussion (Chapter 5), where new insights into how Organic Chemistry instructors provide mechanistic explanations are presented (Chapter 5.2). These findings are intended to contribute further insights from practice to the construction of the instructional mechanistic explanations. Then, the development and implementation is presented (Chapter 5.3.1). Findings from the practical implementation follow (Chapter 5.3.2), focusing on the effects of the developed instructional mechanistic explanations on students' construction of mechanistic explanations.

3. Research Objectives

This dissertation is part of the research project "EYE-OC", funded by the German Research Foundation (grant number: 329801962). The aim of the project was to qualitatively and quantitatively analyze the effectiveness of developed instructional resources that aimed at promoting students' problem-solving when engaged in mechanistic tasks in Organic Chemistry. The aim of this dissertation within the project was to develop and test instructional mechanistic explanations.

As a complement to theoretical considerations and empirical research findings (Chapter 2), and in light of the fact that the influence of instructors on student learning is widely acknowledged and known (Hattie, 2008), the analysis of instructors' mechanistic explanations is used herein to provide a holistic picture of the construction of effective instructional explanations. Thus, instructors' mechanistic explanations will be elicited to develop *instructional mechanistic explanations* that can be implemented in multimedia formats and teaching in Organic Chemistry.

Hence, this dissertation aims to develop and test instructional mechanistic explanations and is guided by the following assumptions:

I. Qualitative analysis of Organic Chemistry instructors' mechanistic explanations provides further insights for constructing instructional mechanistic explanations for Organic Chemistry.
II. Qualitative analysis of students' mechanistic explanations before and after watching tutorial videos with implemented instructional mechanistic explanations provides new insights into how to effectively construct instructional mechanistic explanations for organic chemistry.

In general, there is a gap between research on the effectiveness of instructional explanations and research on the design of tutorial videos (Brame, 2016; Kulgemeyer and

Peters, 2016). This dissertation, as part of the EYE-OC project, contributes to filling this gap by investigating how to construct instructional mechanistic explanations and tutorial videos for mechanistic problem-solving in Organic Chemistry. The evaluation of the videos' effectiveness will further add to the understanding of learning and teaching in Organic Chemistry with instructional (multimedia) resources.

4. Conducted Studies and Methods

Within the EYE-OC project, three studies were conducted (Figure 3). The studies were developed and conducted in close cooperation between researchers from the Leibniz Institute for Science and Mathematics Education (IPN) in Kiel and the Justus-Liebig-University (JLU) in Gießen. (IPN Kiel: Sascha Bernholt, Marc Rodemer, Gyde Asmussen; JLU Gießen: Nicole Graulich, Julia Eckhard, Axel Langner).

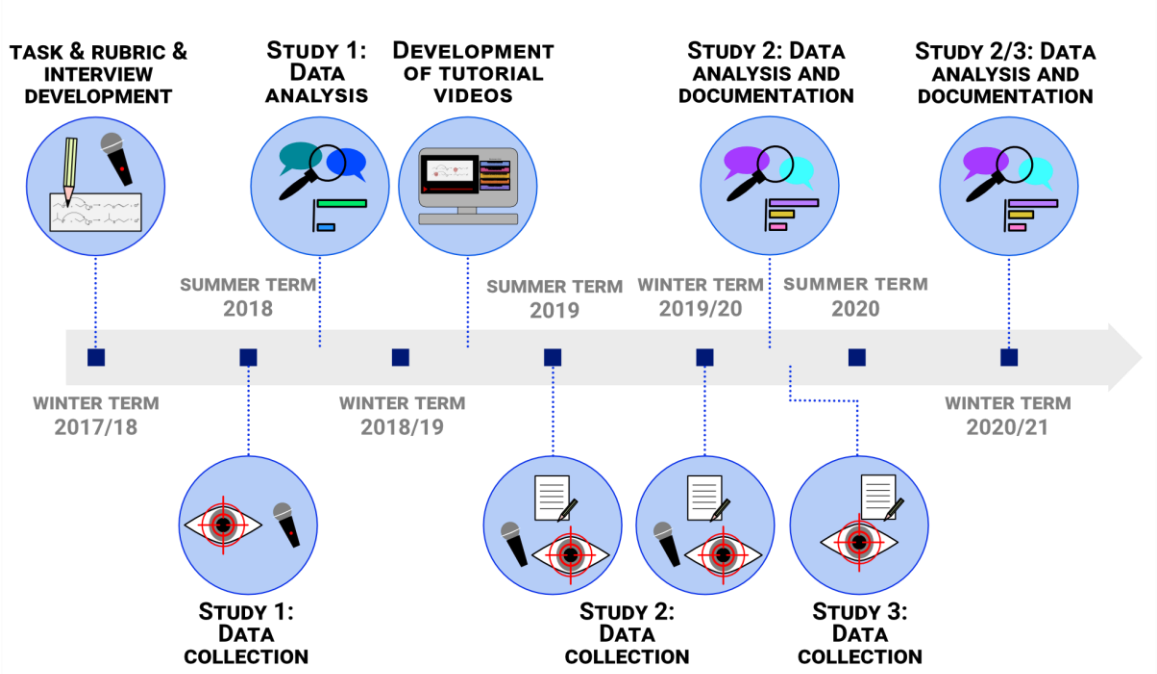

Figure 3: Research design with studies and methods used in the project, the microphone symbol represents qualitative interviews. The project started in the winter semester 2017/18 with the development of case comparison tasks and qualitative interviews. In spring of 2018, the instructional materials for the first study were piloted. The first study was conducted in the summer semester of 2018. The first study used eye-tracking and qualitative interviews as methodological approaches. Over the course of a year, data analysis was conducted and the instructional explanations were developed and implemented in tutorial videos to test their effectiveness on student learning. The instructional materials, including the qualitative interviews and tutorial videos, were piloted in the spring of 2019. The second study was conducted in the summer semester of 2019 and the winter semester of 2019/20. The second study used a mixed methods approach, including eye-tracking and qualitative interviews. Data analysis, including qualitative content analysis, followed. The third study was conducted until the summer semester of 2020. In this study, eye-tracking measures were used to further investigate the perception and processing of highlighting in the designed tutorial videos.

The research design of the studies was in accordance with ethical standards and all participants were informed about their rights and the handling of the data (IRB approval is not a requirement at German universities). Participants were assured that they could have

an opt-out at any time during the data collection process. Written informed consent was obtained prior to each data collection (Appendix 10.1, p. 115; 10.5, p. 130). Within this dissertation project qualitative content analyses of semi-structured interviews were performed as methodological approach. For data analysis, interviews were transcribed verbatim and entered into MAXQDA® coding software (Appendix 10.4,p. 129; 10.8, p. 144). The interviews were conducted in German and translated for publication (translation of the quotes see: Appendix 10.9, p. 145).

To provide a complete picture of the project and the research that complements the findings of this dissertation project, the two studies relevant to this dissertation are described in more detail in the following, including quantitative and qualitative research strands.

Study 1: Decoding Case Comparisons: How Do Different Groups of Expertise Decode Case Comparison with Regard to Visual and Explanatory Behavior?

Different expertise groups were recruited, namely beginner (n = 20) and advanced students (n = 16) as well as experts of Organic Chemistry (lecturers and professors) (n = 10). While the focus of the first study (Figure 4) of this dissertation project was the examination of instructors' mechanistic explanations to gain further insights on the development of instructional mechanistic explanations, the study in parallel aimed to obtain data to analyze the extent to which students' visual behavior is influenced by prior knowledge and the complexity of the representations (see further: Rodemer *et al.*, 2020). Furthermore, the visual behavior of different expertise groups was focused on. The findings were intended to inform ways to visually guide students through the representations, i.e., how visual support can be designed meaningfully, and whether expert eye gazes are suitable as eye movement modeling examples to support students (see further: Graulich *et al.*, 2022). In order to determine which cognitive resources are activated by the participants, another line of research focused on which domain-specific concepts are derived from the structural formulas (see further: Asmussen *et al.*, 2022).

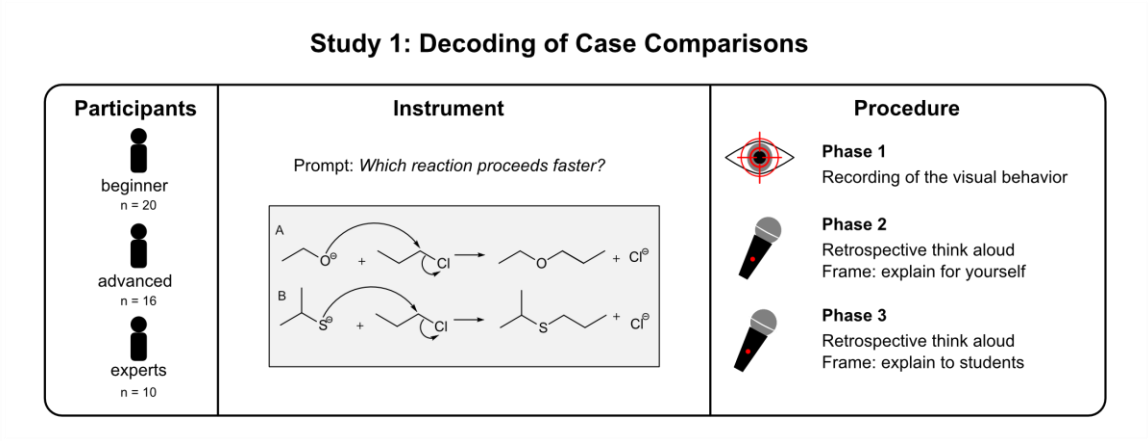

Figure 4: Research design of study 1. Different expertise groups (beginners n=20, advanced students n=16, experts/instructors n=10) were asked to solve case comparison tasks (Instrument) in different phases. First, they were eye-tracked while thinking for themselves (Phase 1), second, they were asked to think aloud (frame = explain for themselves/a colleague) (Phase 2). A third phase was performed only by experts/instructors as they were asked to explain to fictitious students (Phase 3).

Participants and Data Collection

Data from the experts, i.e., the instructors, were relevant to this dissertation. Of the ten instructors who volunteered to participate in the study, nine were male and one was female (no other gender was reported). Seven of the ten instructors were leaders of Organic Chemistry research groups; the remaining three were affiliated with such research groups. All of the instructors were professors or lecturers who regularly taught undergraduate courses following a traditional curriculum. Their teaching experience ranged from 11 to 30 years. The average was 21 years.

During the study, participants were presented with case comparison tasks on a screen while their eye movements were recorded with an eye tracker (Phase 1). Participants had to decide which of two reactions was faster (see Appendix 10.3, p. 123, for sample solutions). After each task, participants were asked to explain their solution in a qualitative semi-structured interview, i.e., retrospective think aloud (Phase 2). In addition, the instructors were asked to explain their solution to fictitious students (Phase 3). Therefore, "*framing*" (Hammer *et al.*, 2005) was used as a lens to elicit variations in explanations.

Framing as a Lens to Elicit Variations in Explanations

An individual's approach to, or activation of, cognitive resources in a situation depends on the framing of the situation, which is influenced by experience but also by explicit instruction (i.e., prompting). Hutchison and Hammer (2010) stated that "[…] *framing shapes how people experience the situation, form expectations, and make choices*" (p. 509). Thus, engagement in constructing explanations may be explained by different instructional frames.

In the first study, the goal was to elicit an *expert frame* that would provide the instructor's problem-solving approach when (successfully) solving mechanistic tasks without instructional context by asking instructors to explain for themselves/think aloud. Changing the explicit instruction to a prompt for an explanation to fictitious students aimed to elicit a *teaching frame* in which explanations are intentionally verbalized for students. This framing was intended to inform how instructors construct their explanations in instruction (as opposed to the *expert frame*).

Data Analysis

A theory-driven coding system was developed that adapted aspects of the coding approach for comparative mechanistic reasoning proposed by Caspari *et al.* (2018), as parts of their coding included the characterization of *causes* and *effects*, a key element for meaningful engagement with mechanistic tasks (Chapter 2.1.2, Appendix 10.4). A multinomial exact test of symmetry was used to compare how instructors used *cause* and *effect* across frames. Pairwise post-hoc comparisons were performed to make inferences about significance.

In addition to identifying instructors' *rationale* in both frames, *explanatory elements* accompanying the *rationales* were characterized. Data-driven codes were developed by constant comparison: the inductive categories of *explanatory elements* included the *description of the process*, the verbalization of *general statements* and rules, and an outline of their problem-solving *approach* (Appendix 10.4, Chapter 5.2.3). Furthermore, a comparison of combinations of *explanatory elements* between the frames was of focus to characterize the sequential use of *explanatory elements* and the embedment of the *rationale* to inform how instructors mediate instructional explanations and support knowledge construction.

The coding of *causes* and *effects* and the coding of *explanatory elements* provided a complete categorization of the instructors' transcripts. Throughout the qualitative analysis, coding schemes were continually discussed among the whole research team to ensure that coding decisions faithfully represented the data. For inter-rater reliability, a random sample of 20% of the data was independently rated by two members of the research team. A Cohen's kappa coefficient of 0.88 was obtained for the *causes* and *effects* coding rubric, and a Cohen's kappa coefficient of 0.93 was calculated for the *explanatory elements* coding rubric indicating high agreement and reliability for both coding rubrics (Rädiker and Kuckartz, 2019).

Insights from the first study (Chapter 5.2 and 8) informed the design of tutorial videos incorporating mechanistic explanations, which were investigated in a second study.

Study 2: Intervention: How Do Students Perceive Purposefully Designed Tutorial Videos on Nucleophilic Substitution Reactions?

Participants and Data Collection

The second study (Figure 5) was designed to evaluate the effectiveness of the developed tutorial videos with the specifically designed instructional mechanistic explanation. In the intervention, 171 undergraduate chemistry students watched three videos on nucleophilic substitution reaction mechanism, as this type of mechanism corresponds to prototypical mechanistic problems in Organic Chemistry. One week prior to the intervention, 12 students completed an in-person pre-interview. In-person post-interviews were conducted during the week following the intervention (see Appendix 10.2, p.120, for interview guidelines and protocol).

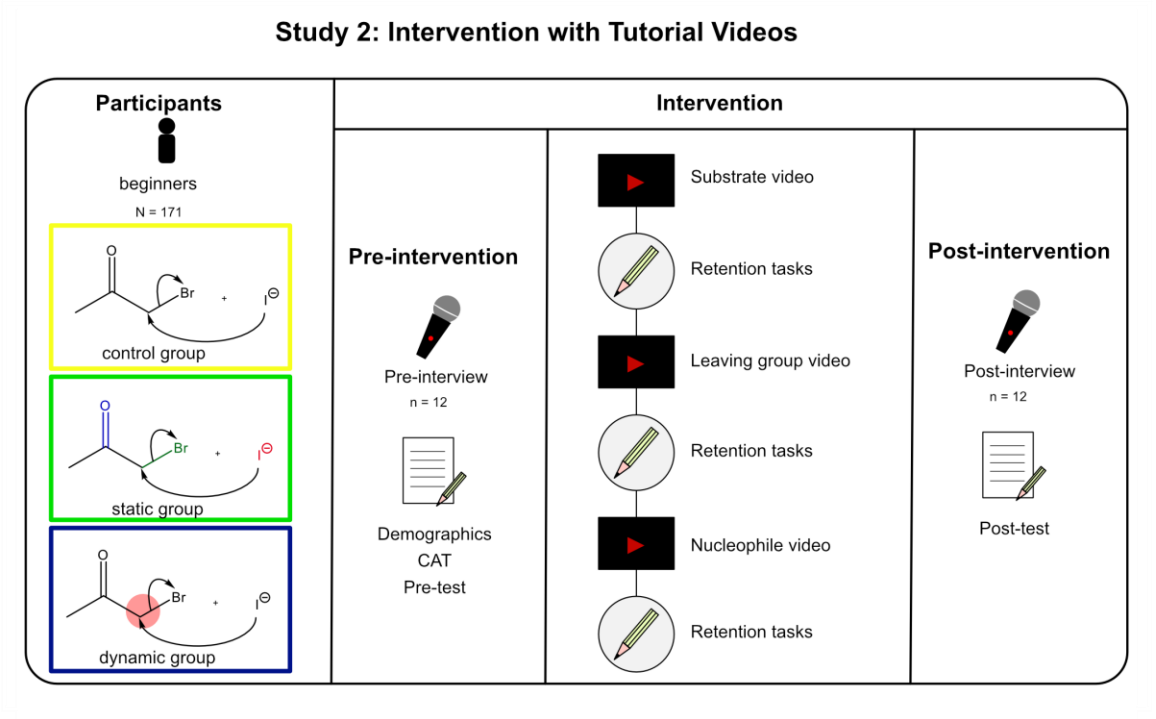

Figure 5: Research design of study 2. At the beginning of the intervention, students (N = 171) were asked to complete a consent and demographic form, a cognitive ability test (CAT), and a pre-test. During the intervention, students watched tutorial videos (a substrate video, a leaving group video, and a nucleophile video) with highlighting according to their group (indicated by the colored frame) on laptops or tablets and completed retention tasks. After watching the videos, students completed a post-test. Of the students (N =171), twelve students participated in the pre- and post-interviews.

In the intervention study, the tutorial videos were tested to determine their impact on students' learning. Qualitative analyses focused on how students processed and understood the implemented instructional mechanistic explanations, i.e., if the modeled reasoning steps in the instructional explanation would be included in the students' explanations (Chapter 5.3.). Figure 6 shows a case comparison task that was used in the

pre- and post-interviews (see Appendix 10.7, p. 140, for further interview tasks). It corresponds to the type of reaction and concepts covered in the tutorial videos.

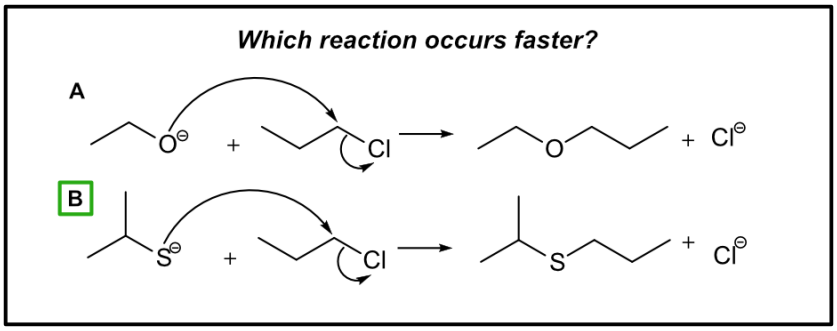

Figure 6: Case comparison task used in the pre- and post- interviews (correct answer is highlighted – however, it was not highlighted for the students in the interview). [Reprinted with permission from [Eckhard, Rodemer, Bernholt and Graulich (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning *J. Chem. Educ*. 2022, 99, 6, p.2235; https://doi.org/10.1021/acs.jchemed.2c00076] Copyright © 2022. Published by American Chemical Society and Division of Chemical Education, Inc.]

The quantitative study aimed at providing empirical evidence for the effectiveness of different highlighting techniques (see further: Rodemer *et al.*, 2021).

Data Analysis

To allow for reliable inference of student assumptions, a deductive coding system was developed, structured by the five reasoning steps implemented in the videos (Appendix 9.3) (Saldaña, 2016). For inter-rater reliability, two members of the research team independently coded a random sample of 20% of the data. A chance-corrected kappa coefficient (Brennan and Prediger, 2016) of 0.92 was calculated, indicating high agreement and reliability (Cohen, 2016; Rädiker and Kuckartz, 2019).

5. Results and Discussion

In the following chapter, the assumptions and the guiding question of the dissertation are addressed in order to conclude how instructional explanations should be designed to support students' construction of mechanistic explanations in Organic Chemistry. First, the main findings of the qualitative analysis of Organic Chemistry instructors' mechanistic explanations are presented and discussed (Chapter 5.2), complementing the reviewed theoretical and empirical findings in Chapter 2. Then, the construction of the instructional mechanistic explanation for the implementation in the nucleophilic substitution videos is presented. Next, the main findings of the second study are shown and discussed in order to examine how the designed instructional mechanistic explanations were processed by students (Chapter 5.3). Quotes from participants are taken from the publications unless otherwise noted (cf. Chapters 8, 9).

5.2. NEW INSIGHTS INTO HOW INSTRUCTORS CONSTRUCT MECHANISTIC EXPLANATIONS TO INFORM THE DEVELOPMENT OF INSTRUCTIONAL MECHANISTIC EXPLANATIONS

In the context of chemistry, instructors were shown to have an important role in facilitating the construction of scientific explanation, i.e., by influencing the translation between representational levels (macroscopic, submicroscopic, microscopic) (Stieff *et al.*, 2013; Becker *et al.*, 2015; Popova and Jones, 2021) and argumentation behavior through different facilitation moves (Stanford *et al.*, 2016; Liyanage *et al.*, 2021). Investigating how Organic Chemistry instructors construct mechanistic explanations is expected to provide further insight into how to develop instructional explanations in Organic Chemistry based on two premises: first, Organic Chemistry instructors, as domain experts, are better able to include key elements, i.e., such as cause-effect relations and important concepts, in their explanations according to their subject matter knowledge (van Driel *et al.*, 2014). Second, Organic Chemistry instructors possess pedagogical content knowledge, i.e., they are able to transform subject matter knowledge and skills for instructional contexts to promote active knowledge construction as teachers (Shulman, 1986; DeFever *et al.*, 2015; Popova and Jones, 2021).

According to assumptions of Cognitive Psychology Research, instructors *as experts* possess higher order and organization of knowledge structures as well as greater conceptual knowledge (Chi, 2006). In this regard, DeFever and Bhattacharyya (2015) compared novice and expert problem-solving approaches in chemistry with respect to knowledge organization: "*In contrast* [to experts]*, novices get mired in these surface-level*

features, often to the point of overloading their short-term memories. Furthermore, these differences in perception and knowledge organization hinder novices' abilities to effectively reason with the facts, especially in cases [such as reasoning through mechanistic tasks] *where information from multiple sources must be weighed against each other in order to make a well-reasoned decision.*" (DeFever *et al.*, 2015, p. 416). Thus, the cognitive abilities of experts, i.e., improved working memory processing, support successful problem-solving of complex problems (Chi, 2006) such as mechanistic tasks. Experts are also known to fluently identify and perceive relevant information from representations, and to relate appropriate and domain-relevant information accordingly (Chi *et al.*, 1981; Kozma and Russell, 1997; Emhardt *et al.*, 2020). Research in Chemistry Education has also shown that experts are better than novices at identifying structural features relevant to mechanistic tasks (Kozma and Russell, 1997; Galloway *et al.*, 2018). Moreover, in the field of Organic Chemistry, experts were found to better be able to integrate multiple and relevant variables to predict the outcome of a reaction (Kraft *et al.*, 2010). Given that expert reasoning is further associated with "*well-reasoned decisions*" (DeFever *et al.*, 2015, p. 416), an analysis of how instructors as experts construct mechanistic explanations, will inform the development of instructional mechanistic explanations.

The influence of instructors and their mediation *as teachers* in support of students' mechanistic reasoning is highlighted in Chemistry Education Research. Talanquer (2018), for example, stated "*Chemistry instructors at all educational levels should foster students' ability to spontaneously and productively apply chemical mechanisms in their sense-making and meaning-making activities regardless of the context*" (Talanquer, 2018, p. 1906). Although this points to instructors as lynchpins to mechanistic reasoning, not much is known about how instructors mediate mechanistic explanations in instruction and what students take away from it. Indications are given by a study of Moreira and colleagues (2019) suggesting that students adapt to their instructors' mechanistic explanations (Moreira *et al.*, 2019). Their study analyzed an instructor's explanations of mechanisms and the influence on students' explanations. During the observed lesson, the instructor emphasized *simple causal explanations*. Analysis revealed that after the lesson, students tended to construct *simple causal explanations* from both directions (i.e., from simpler and more sophisticated modes of reasoning to simple causal explanations (Sevian and Talanquer, 2014)). Hence, the instructor's modes of reasoning, i.e., her included simple cause-effect relations, had an influence on students' constructed mechanistic explanations (Moreira *et al.*, 2019). Beyond these findings, little is known about how instructors construct their mechanistic explanations in instruction. In accordance with the research objectives and the first assumption of this dissertation, the qualitative analysis of

Organic Chemistry instructors' mechanistic explanations will provide further insights into the construction of instructional mechanistic explanations for Organic Chemistry. Therefore, the main findings of study 1 are presented in the following. These findings are part of the paper presented in Chapter 8.

5.2.1. How Do Instructors Make Use of Causes and Effects When Explaining Case Comparisons in an Expert Frame and in a Teaching Frame?

When solving mechanistic tasks, students often reason with unproductive heuristics (e.g., verbalisms) or with explicit surface features of representations, neglecting causal relationships (see Chapter 2.1.3). Therefore, the analysis of instructors' mechanistic explanations focused on their use of (implicit) *causes* and *effects*. It was examined to what extent they elaborated, i.e., which grain size they used, and whether they included the electronic structure and its change (cf. Chapter 8, Appendix 10.4). In particular, it was of interest to determine whether *causes* and *effects* were verbalized in relation to each other, in order to obtain indications of how cause-effect relations are implemented in mechanistic explanations and to draw conclusions for the construction of instructional mechanistic explanations.

As Figure 7 shows, the distribution and combination of *causes* and *effects* in the instructors' rationales of their explanations reveal differences between the frames. While the rationales in the expert frame often included comparisons of explicit, descriptive features, the rationales in the teaching frame more often included implicit aspects on a deeper grainsize, which often also included the (change of the) electronic structure (Figure 7).

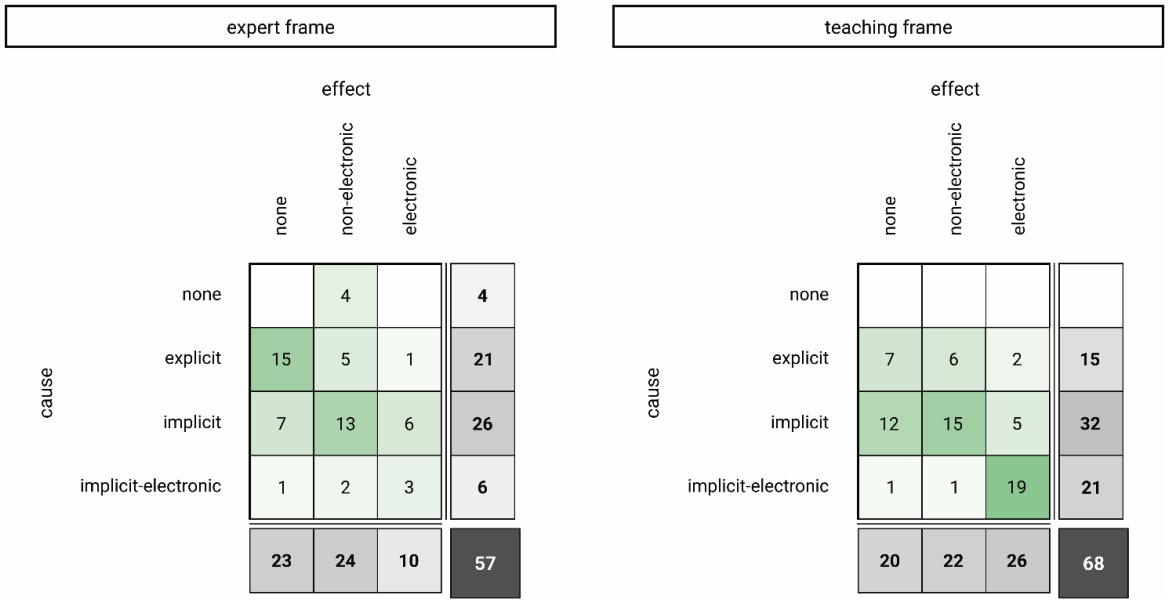

Figure 7: Distribution and combination of *cause* and *effect* codes in the expert frame (left) and in the teaching frame (right); the darker the color, the more codes were identified. Green tiles represent the combination of *cause* codes (y-axis) and *effect* codes (x-axis), *e.g.*, in the expert frame (left) 5 explicit causes were stated in combination with non-electronic effects. Grey tiles represent the sum of each code category. Total number of rationales of ten instructors solving four tasks in each frame: expert frame = 57; teaching frame = 68. [Reproduced from (Eckhard *et al.*, 2022, p. 85) with permission from the Royal Society of Chemistry]

In the *expert frame* the instructors provided a total of 57 rationales when asked to solve the case comparisons (Figure 7, left). The *causes* used in these rationales differed in the extent to which the instructors used implicit information, such as implicit properties. In order to make a claim about which of the two reactions proceeds faster, one would expect *causes* and *effects* to be verbalized in relation to each other. Therefore, it was analyzed if complete cause-effect rationales were formed. Results show that almost half of the rationales were incomplete (4 rationales without *causes*, 23 rationales without *effects*).

In the *teaching frame*, instructors used a total of 68 rationales to explain their reasoning (Figure 7, right). As was the case in the expert frame, *causes* and *effects* were not always mentioned together. As opposed to the expert frame, each rationale included a *cause*. However, in the teaching frame, the *effects* of the mentioned *causes* were missing in 20 out of 68 rationales, so that almost a third of the instructors' cause-effect rationales can be considered incomplete.

Cause and effect combinations

In the *expert frame***,** the most common combinations of *causes* and *effects* found in rationales (Figure 7, left) show that instructors often relied on *explicit causes*, i.e., used structural features to support their claim without mentioning an *effect* of a structural cause (combination count: 15). This finding can be exemplified looking at instructor Franklin's

explanation of task 4. In his statement, he first described the type of reaction and then referred to the backbones of the substrates in a bullet-point fashion.

Instructor Franklin: *S_N1 substitution. Tertiary substrate versus twice benzylic tertiary substrate. B is faster by orders of magnitude.* (Task 4, expert frame)

The instructor compared the representational features (tertiary and secondary substrate) without reference to implicit properties (such as electron donation via inductive effects). Hence, his rationale entailed an *explicit cause*. Further, he verbalized a qualitative difference, e.g., "*is faster*" as a claim, which he linked to the explicit structural differences. He did not state further effects of structural causes, such as charge weakening. The verbalization of *causes* without mentioning *effects* on the course of the reaction, i.e., changes, as exemplified by the statement of instructor Franklin, was identified in 40% of the rationales in the *expert frame*.

In addition to explicit structural differences, implicit structural properties were mentioned in 56% of the rationales. Most often (Figure 7, left), these *implicit causes* were used in combination with *non-electronic effects*. These *non-electronic effects* verbalized how a structural cause affected the course of the reaction without reference to the level of electrons, i.e., stabilization was often stated as a *non-electronic effect*. Instructor Evans' explanation illustrates the combination of *implicit causes* with *non-electronic effects* in his rationale.

Instructor Evans: *Yes, it's about splitting off from a leaving group and then a secondary and tertiary substrate form. In addition, the tertiary will almost certainly go better because it is better stabilized through inductive effects*. (Task 1, expert frame)

It is shown that Evans acknowledged the explicit difference of the backbones (tertiary and secondary substrate). He related the inductive effects of the tertiary alkane as an implicit property (*implicit cause*) and mentioned the resulting increase in stabilization. His explanation was not coded as *implicit electronic cause*, as a reference to the level of electrons was missing, e.g., the positive inductive effects resulting from electron donation of the methyl groups. Instructor Evans further quickly generated his explanation by using a heuristic in terms of reliance on the constitution of the backbones of the substrate. Talanquer (2013) stated within this regard of expert chemists, that chemists "*rely on the thoughtful application of a variety of empirical generalizations used as heuristics or rules-of-thumb to make quick decisions*" (Talanquer, 2013, p. 836). Thus, by quickly generating a claim based on a heuristic that was useful to him, instructor Evans demonstrated an expert-like manner.

In the *expert frame*, the instructors' explanations were mostly characterized by making comparisons based on explicit structural features and naming implicit structural properties to support their claim, without referring to the electronic level or inferring effects of structural causes. The findings of "abbreviated" use of *causes* and *effects* (without a reference to the electronic structure) could easily be interpreted as a lack of sophistication, as it mirrors the findings from student approaches (Chapter 2.1.3). However, it is more likely that the instructors' verbalization of *explicit* and *implicit causes* (neglecting the electronic structure and its influence on the course of the reaction) is related to their expert response behavior to the prompt of the frame. Their explanations are therefore precise, avoid digression and neglect further elaboration on the electronic level, as this could be redundant for the addressees. This corresponds to giving *minimal explanations* and taking into account the prerequisites of the addressees (Carroll*, et al.*, 1987; Renkl*, et al.*, 2006). That is, they anticipate the existing knowledge of the addressee (themselves or a colleague, also an expert).

In the *teaching frame* (Figure 7, right dark green tile), the most frequent cause-effect rationale included a combination of *implicit-electronic causes* with *electronic effects*. The excerpt from instructor Davis illustrates this finding. Instructor Davis referred to the explicit difference in the different backbones of the products (*tert-butyl* carbocation vs. diphenylethyl carbocation) and inferred implicit electronic properties. He considered the electronic structure and considered this implicit electronic property as a *cause* by explaining that the *p*-orbitals can overlap and donate electron density to the empty *p*-orbital of the cation (*implicit electronic cause*). He further verbalized how this leads to delocalization of the positive charge and sharing of the electron deficiency, which was categorized as an *electronic effect*.

Instructor Davis: […] *The second reaction is faster. This is due to the stability of the generated cation. The biphenyl substituted cation is more stable than the tertiary butyl cation, which we see in reaction A. And this is due to the two phenyl substituents. They contribute to the stability of this cation by donating electron density of the p-orbitals. The empty p-orbital of this cation [in B] can overlap with the p-orbitals of both phenyl rings and thus… positive charge is delocalized over 13 C-centers [carbon atoms]. Then each of them [the carbon atoms] has to carry only a 13th of the electron deficit load. Yes, this is what makes this cation so stable*. […] (Task 4, teaching frame, excerpt)

In addition to naming concepts and implicit properties in his rationale, instructor Davis elaborated on the electronic level, such as the ability of phenyl substituents to donate electron density of the *p*-orbitals. He mentioned the delocalization and charge weakening

(*electronic effect*) that accounts for the stability of the diphenylethyl cation in his verbalization of the *effect* of such a *cause*. In his rationale, he included the origin of stability by reference to the electronic level and thereby gave a more profound meaning to the term stable. A term used by many students in their problem-solving approach without a deeper conceptual understanding (Caspari *et al.*, 2018; Deng and Flynn, 2021). Instructor Davis explanation exemplifies that in rationales combining *implicit-electronic causes* and *electronic effects*, domain-specific concepts and implicit properties were not only used as catchwords or in an abbreviated form, but were explained in a process-oriented way with regard to the (change of the) electronic structure. However, not all of the rationales in the teaching frame entailed a cause-effect rationale regarding the electronic structural properties and their changes, which would correspond to a high complexity of a relation. In terms of the complexity of relations, Caspari and colleagues (2018) stated "*A more complex relation [with an electronically justified cause and effect] is not necessarily any better (or worse) than a less complex one. The advantage of a less complex relation is that it can be more easily communicated than a complex relation and enables faster decision making*" (Caspari *et al.*, 2018, p .1130). Hence, when instructors use less complex cause-effect rationales in their explanations – either in the *expert frame* or in the *teaching frame* – they could have aimed at faster decision making or providing more accessible explanations.

The use of *implicit causes* in combination with *non-electronic effects* was the second most common combination in the *teaching frame*. In addition, *implicit causes* without reference to electronic properties and interactions were used in almost half of the rationales in the *teaching frame*. Thereby, causes were often expressed as mere labels of properties, i.e., rather as verbalisms and buzzwords (e.g., "*is a weak base, therefore* [...]"). Research findings show that students tend to rely on verbalisms and tend to memorize these without having a deep understanding of the verbalism (e.g., Bhattacharyya, 2008). Hence, students may adapt vague explanations in instructional contexts. Further, abbreviating explanations in instructional settings to, for example, "*good or bad"* leaving groups or "*strong or weak*" acids may result in learners remaining in dualistic thinking rather than considering multiple variables. This could result in the use of buzzwords as empty envelopes, that mask the lack of deep understanding of chemical concepts (Popova and Bretz, 2018). Therefore, instructional mechanistic explanations should avoid buzzwords for addresses with low prior conceptual knowledge. Rather, instructional mechanistic explanations should involve reasoning with properties to support a deep understanding of chemical concepts, as exemplified by instructor Davis, whose explanation addressed this in terms of giving a deeper meaning to the term stable.

As often as *implicit causes* were combined with *non-electronic effects* was the combination of *implicit causes* without an effect, i.e., inference of structural properties without describing the influence of structural properties on the reaction course in the *teaching frame* (Figure 7, right). The instructors' final claim to the tasks was often a purely qualitative statement, e.g., "*lower basicity and higher stability*" (Instructor Carter, Task 3, teaching frame), rather than describing the effect on the course of the reaction and making a claim about energy as suggested by Philosophy of Organic Chemistry (Goodwin, 2003). Instructors often remained vague about the source of this qualitative difference, and did not address the effect of a structural cause and related it to the energetic course (e.g., energetic lowering of the transition state). In instructional contexts and explanations, simply stating qualitative differences could result in students memorizing these differences (or, as aforementioned, these buzzwords) without gaining a greater understanding useful for problem-solving of complex or unknown tasks. Intentional implementation of the effect on structural change in instructional explanations could fill in the reported missing link of students between the structural cause and the claim about energy (Caspari *et al.*, 2018; Macrie-Shuck and Talanquer, 2020).

The main results show that instructors changed their explanation, i.e., use of *causes* and *effects* according to their framing. In the following it is presented if and how a change in the elaboration of the use of causes and effects took place due to the frame shift.

5.2.2. How Does the Use of Causes and Effects in Instructors' Mechanistic Explanations Change from an Expert Frame to a Teaching Frame?

In order to identify changes in explanations of how instructors might intend to support students' knowledge construction in the instructional setting (*teaching frame*), the frequency distributions of *cause* and *effect* codes from both frames were analyzed. In doing so, it was analyzed which codes refer to the same concept or content in both frames and which codes differ, that is, how the use of *cause* and *effect* might vary across frames. Altogether, the results show a tendency towards an increase in grain size in both *cause* (Figure 8, left) and *effect* codes (Figure 8, right) from the *expert* to the *teaching frame*. An increase in the use of *causes* and *effects* (Figure 8), and the use of multiple rationales in the *teaching frame* with different conceptual approaches was also identified (Appendix of Chapter 8).

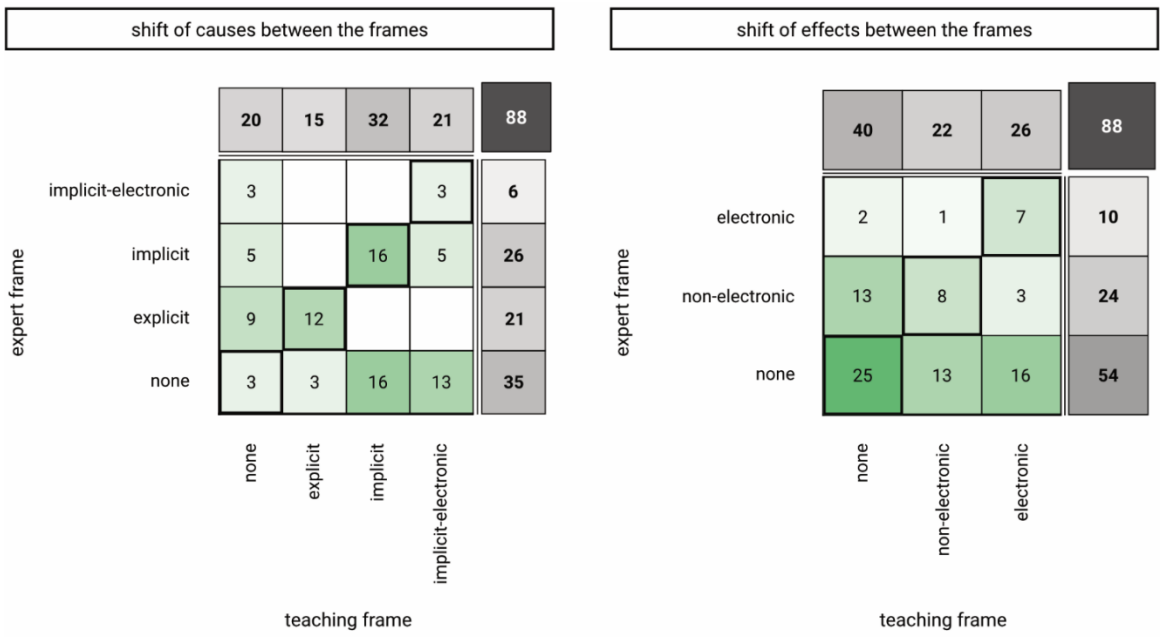

Figure 8: Cross tables representing the distribution of *cause* codes (left) and *effect* codes (right) for both frames. The tiles of the cross table represent a match (thicker edged, diagonal tiles) or a shift of a code between the frames (y-axis: *expert frame*, x-axis: *teaching frame*). [Reproduced from (Eckhard *et al.*, 2022, p. 89) with permission from the Royal Society of Chemistry]

Qualitative content analysis revealed differences in the completeness of the cause-effect rationales – as well as differences in the grain size of *causes* and *effects* – when regarding instructors' frame shift. It was found in the *expert frame* often instructors who verbalized *explicit causes* without an effect or with *non-electronic effects* changed to verbalizing rationales including *implicit-electronic causes* with *electronic effects* and *implicit causes* without resulting effects in the *teaching frame* (e.g., instructor Robinson, compare Chapter 8).

In addition, in the *teaching frame* instructors tended to use multiple rationales, i.e., multiple conceptual approaches to support their claims (Appendix of Chapter 8). Thereby, the claim about energy has often been made by two conceptual approaches: 1) the capacity of a leaving group to distribute charge via resonance, and 2) a statement about acidity. This is exemplified in instructor Robinson's explanation in the *teaching frame*. In contrast to the *expert frame*, where he combined one *explicit cause* with a *non-electronic effect*, in the *teaching frame* instructor Robinson verbalized implicit-electronic properties for mesylate being the more favorable leaving group and described an effect of that structural cause including interactions on the electronic level. Further, he inferred a conceptually different rationale to his first rationale by mentioning the acid/base properties of the leaving groups (implicit cause).

Instructor Robinson: *Right. If we compare the reactions here, the difference is the leaving group. We simply have an amine at the top [reaction A] and mesylate at the bottom*

[reaction B]. This means that even if both reactions run by a S_N2 mechanism, we compare the different quality of the leaving group and thus we see how stabilized the leaving group is when it is split off. This means that we have the amide at the top [reaction A], accordingly, NH_2 minus, while we have the mesylate at the bottom [reaction B]. In the lower case, the negative charge can be distributed over all three oxygen atoms by simply flipping over the electron pairs. That means there is a strong mesomeric effect present and as you know, charged species are… the more you can distribute their charge… or the more atoms you can distribute it to, the more favorable. *This can also be directly correlated with the pKa value. That means, the stronger the corresponding acid to the anion, the better the anion can be considered as leaving group. And if you now look at the pKa value of the amine and compare it with the corresponding sulfonic acid… then you would immediately see that the amine is much less acidic, because amines react as a base after all and from this you can deduce that mesylate is the better leaving group and should be faster in B.* (Task 2, teaching frame)

Regarding instructor Robinson's explanation, the example shows how his two rationales are linked. He provided an explanation of how acid/base strength is related to mesomeric effects. Not only did he provide two conceptual approaches, but he also showed how these are related through electronic structure, e.g., capacity to accommodate charge, which was often found when instructors used multiple rationales (Appendix of Chapter 8).

In summary, the findings on the change in instructors' use of *cause* and *effect* show that more elaborated cause-effect rationales were stated in the *teaching frame* than in the *expert frame*. This finding indicates the adaptability of instructors to consider the prerequisites (either themselves or colleagues as experts → *expert frame*, or students → *teaching frame*) and to adjust their explanation depending on the framing. In the *teaching frame*, it appears that they often interpreted the prompt to explain to a student as a further elaboration of what they may not have explicitly verbalized in the expert frame. This is reflected in an increase in the number of rationales, in the more frequent establishment of causal relations and through the verbalization of a deeper grain size. The consideration of *causes* and *effects* on a deeper grain size in the *teaching frame* further highlights the tendency of instructors to move away from descriptive explanations, as implicit properties, the electronic structure of entities and its change in the course of the process were stated. This could be interpreted as an effort to support students in inferring what is implicitly encoded in the representations and process-oriented reasoning with their (instructional) explanations in the *teaching frame*. Further, an increase in the use of *causes* and *effects* could be observed from the *expert frame* to the *teaching frame*, through instructors building multiple cause-effect rationales in the *teaching frame*. The latter seems promising in terms

of thinking about how to provide students with different conceptual approaches to a problem. The findings of a study by Bodé and colleagues (2019), in which students' problem-solving of a mechanistic task was investigated, show that incorrect claims were often made when only few connections between concepts had been made (Bodé *et al.*, 2019). This suggests that verbalizing multiple conceptual approaches through instructional mechanistic explanations that include connections between concepts, e.g., electronic structure (as instructor Robinson did when explaining task 2 in the teaching frame), could support strengthening connections between concepts and thus successful problem-solving.

In the *teaching frame*, it was also found that in one-third of the rationales, verbalizing complete causal relationships was neglected in terms of verbalizing structural causes in combination with their effects, even though the instructors were targeting their explanations to beginner students. Mentioning such causal relationships can be considered crucial for students in terms of successfully explaining (unknown) mechanisms (Machamer *et al.*, 2000; Cooper, 2015; Caspari *et al.*, 2018) (Chapter 2.1.2). The latter points to the need to be aware of the target groups' prerequisites to make instructional explanations effective for learners (Wittwer and Renkl, 2008).

To inform the construction of instructional mechanistic explanations about how instructors intend to support student knowledge construction and cognitive activation, it was further of interest how instructors combine their rationale with additional *explanatory elements*, especially when they target their explanations to students.

5.2.3. How Is the Rationale Combined with Additional Explanatory Elements in the Different Frames?

Inductive content analysis of instructors' explanations revealed three additional categories of *explanatory elements* besides the *rationale*, i.e., *process description*, *general statement*, and *approach* (Figure 9). Findings reveal an increase from the *expert frame* to the *teaching frame* when comparing the use of *explanatory elements*. The qualitative content analysis further suggests that instructors tend to include additional elements to support students' understanding within the *teaching frame*. Assuming that the instructors adapted their initial explanations by shifting to the *teaching frame*, this is not surprising.

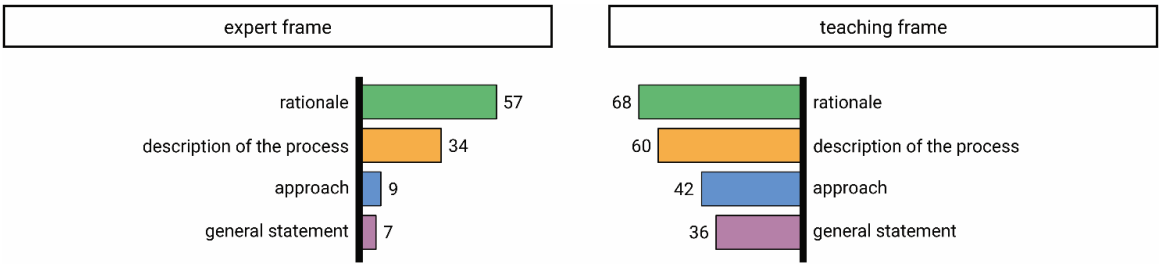

Figure 9: Identified *explanatory elements* in instructors' explanations for 40 tasks (n=10 instructors, solving 4 tasks) in the *expert frame* (left) and for 40 tasks (n=10 instructors, solving 4 tasks) in the *teaching frame* (right). [Reproduced from (Eckhard *et al.*, 2022, p. 92) with permission from the Royal Society of Chemistry]

To inform the construction of instructional explanations in terms of combining *explanatory elements* and embedding of the *rationale,* the combination of *explanatory elements* and their sequential use further was analyzed (Figure 10).

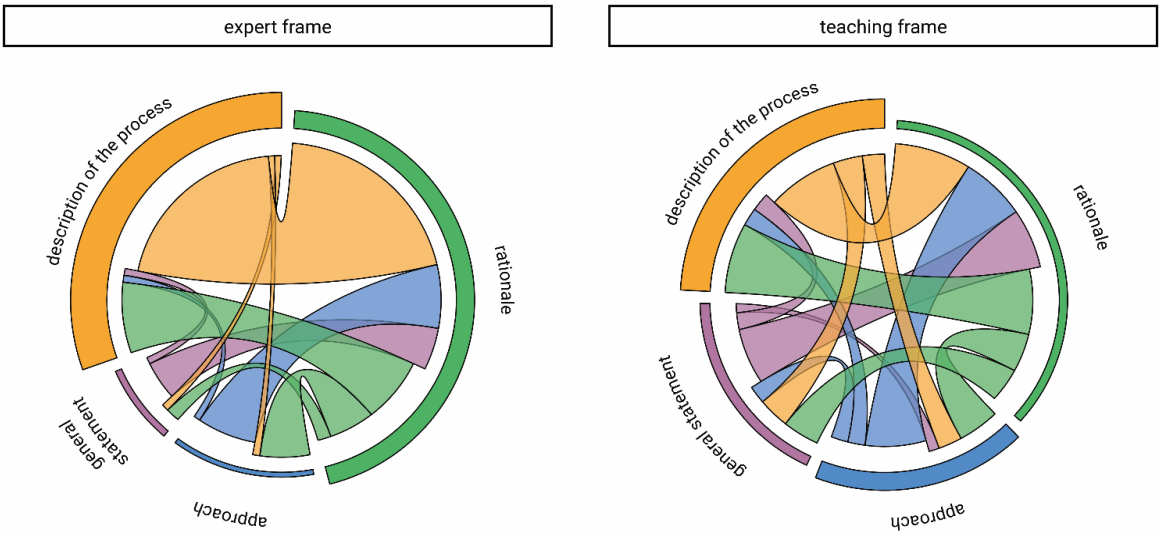

Figure 10: Relative numbers of transitions between *explanatory elements* in the *expert frame* (left) and in the *teaching frame* (right). The proportions of the outermost ring indicate the relative frequency of the reference to an *explanatory element*. The height of the outermost ring (node) indicates how often an explanation was started with the respective *explanatory element*. The width of each chord represents the frequency of transitions made between respective *explanatory elements*; indented chords symbolize a transition from one *explanatory element* to another. [Reproduced from (Eckhard *et al.*, 2022, p. 92) with permission from the Royal Society of Chemistry]

As shown in Figure 10, the frequent use and accompany of the *rationale* with the *description of the process* was evident in both frames. In the *teaching frame*, this mentioning and combination of a *rationale* with a *description of the process* in an instructional explanation could be beneficial for students as it goes beyond a static description of entities and highlights the changes in a dynamic manner. Further, in the *teaching frame*, *general statements* and *approaches* more often accompanied the *rationale*, and more transitions between *explanatory elements* could be detected in instructors' explanations (Figure 10). In addition to the *description of the process*, the problem-solving *approach* was often used to begin an explanation in the *teaching frame*

(Figure 10, right, height of blue node). This can be exemplified looking at instructor Miller's explanation for task 2 in the teaching frame.

Instructor Miller: *Well, to determine which reaction is faster, we have to rely on the quality of the leaving group.* […] (Task 2, teaching frame, approach)

Instructor Miller began by discussing how one might *approach* the question of trying to determine which of the two reactions proceeds faster. His next step was to make a *general statement* by relating the stability of a leaving group to the stabilization of the negative charge.

Instructor Miller: […] *And it is like this: the more stable a leaving group, the better the negative charge can be stabilized*. […] (Task 2, teaching frame, general statement)

Then he went on to give an *approach* to finding out which of the leaving groups is better stabilized, i.e., by regarding the explicit features of the structural formulas.

Instructor Miller: […] *And you can tell this either by looking at the structure and recognizing that* […] (Task 2, teaching frame, approach)

He then explained his reasoning by acknowledging the (de)localization of charge. In his explanation, he guided a fictitious student through the task by explicitly explaining a strategy for solving the tasks. He used direct address several times (*we*/*you*). He showed an adaptation of the language level and personalization in his explanations (compared to the *expert frame*) that may have had the goal of promoting cognitive activation of his (fictitious) students (Kulgemeyer, 2019). The use of *approaches* may have been a way for instructors to guide learners with specific prompts, which is known to increase cognitive activation (Wittwer and Renkl, 2010; Kulgemeyer, 2019). However, instructors' categorized *approaches* differ qualitatively among them. While some of the verbalized *approaches* may be beneficial to learners by providing the concepts or trains of thought, others may not be, as they may trigger pattern recognition based on representational features ("*looking at the structure and recognizing that*...") and thus encourage unproductive heuristic reasoning based on surface features. Within that regard, Galloway and colleagues (2018) stated "*Students need to be taught how to read organic reactions, what to pay attention and why, […]. For example, if we want students to learn to think mechanistically and demonstrate such thinking, then they need to be able to identify areas of high and low electron density*." (Galloway *et al.*, 2018, p. 363f.). Therefore, as the analysis of instructors' use of *explanatory elements* shows, when developing mechanistic explanations for instruction, *approaches,* in general and those that include "*what to pay attention to and why"* (Galloway *et al.*, 2018, p. 363) could be beneficial to students'

problem-solving. Hence, an instructional mechanistic explanation could support students by providing an *approach* for how and where to infer implicit properties from the explicit features of a mechanism.

In the *teaching frame,* instructors often used *general statements*. This is known to support knowledge construction through structuring, i.e., segmentation (Kulgemeyer, 2019; Mayer, 2021). It was found that the instructors would often first propose a *general statement* and then give an example of how the *general statement* was related to the task at hand. This can be illustrated by instructor Evans' statement: "*That is, the reactivity for nucleophilic substitution reaction basically increases from primary to secondary to tertiary in the case of S_N1*."(not mentioned in the paper) or instructor Davis' statement for Task 4, where he mentioned a *general statement* about electrophilicity and nucleophilicity: "*Everything is always based on the principle that an electrophile reacts with a nucleophile. And if the electrophile is more electrophilic, the reaction is faster. If the nucleophile is more nucleophilic, the reaction is faster. This can be applied to all the reactions we are comparing here in the same context."* (Task 4, teaching frame, not mentioned in the paper). This approach refers to a rule-example strategy and has been shown to promote the learning of content knowledge (Tomlinson and Hunt, 1971; Seidel *et al.*, 2013). Nevertheless, the tendency of students to overgeneralize general statements and rules is also documented, for example, when classifying reactions (Stains and Talanquer, 2008) or when applying the octet rule (Taber, 1998; Luxford and Bretz, 2014). Overemphasizing *general statements* in instructional settings and explanations may encourage reliance on rule-based reasoning that focuses on a single variable in cases where multi-variable reasoning would be required (Kraft *et al.*, 2010; Talanquer, 2014). Consequently, as the instructors' explanations revealed, *general statements* provide structure to explanations. However, to support learning of content knowledge while supporting multivariable reasoning (rather than blind reasoning with single variables and rules), *general statements* and rules should be carefully implemented in instructional mechanistic explanations, regarding the prerequisites of the target group.

Even though more *explanatory elements* were found in the *teaching frame* and relate to instructors' effort to support students, the mere and multiple naming of *explanatory elements* should not be regarded as being beneficial in itself. Qualitative differences within the codes could be identified (e.g., in the verbalization of *approaches*), which may also influence the effectiveness of explanations for students with regard to their need of support.

In summary, the results show that instructors are engaged in adapting their explanation according to the frame, which illustrates their ability in elaborating their mechanistic explanation according to the context and addresses (cf. Chapter 8).

In this chapter, implications for the construction of instructional explanations were derived by linking the results of instructors' explanations with known findings from Chemistry Education Research on students' problem-solving approaches. These implications complement the review of theoretical and empirical findings from different research perspectives in Chapter 2, and lead to the construction and testing of instructional mechanistic explanations discussed in the next chapter.

5.3. NEW INSIGHTS INTO WHAT UNIVERSITY STUDENTS TRULY LEARN WHEN WATCHING TUTORIAL VIDEOS WITH PURPOSEFULLY DESIGNED INSTRUCTIONAL MECHANISTIC EXPLANATIONS

5.3.1. Construction of the Instructional Mechanistic Explanation

The instructional mechanistic explanation in the tutorial videos regarded case comparisons tasks of nucleophilic reaction mechanisms, which led to the development of three videos: a substrate video, a leaving group video and a nucleophile video. Taking into account the perspectives of Philosophy of Science on well-reasoned explanations for Organic Chemistry (Machamer *et al.*, 2000; Goodwin, 2003) and frameworks characterizing mechanistic reasoning in chemistry (e.g., Sevian and Talanquer, 2014; Becker *et al.*, 2016; Caspari *et al.*, 2018), *aspects* (entities, activities, organization and interaction, linking structure and energy) and *key elements* (cause-effect relationships, process orientation, consideration of multiple variables) were derived (Chapter 2.1.1 and 2.1.2) that were included in the instructional mechanistic explanation. With the target group of Organic Chemistry students in mind, aspects of Instructional Research were discussed and combined with findings from Chemistry Education Research in order to increase the effectiveness of the instructional mechanistic explanation for learners (e.g., regarding prerequisites, avoiding digressions when explaining mechanisms, and promoting knowledge construction) (Chapter 2.1.3 and 2.1.4). In the construction of the instructional mechanistic explanations, these considerations were related to the considerations of instructional design, as the delivery format, i.e., multimedia design, influences effectiveness (Chapter 2.1.5). Again, the prerequisites of the target group were taken into account and the format of videos was chosen accordingly to deliver the instructional mechanistic explanation (Mayer, 2021), e.g., to strengthen the link between representations and implicit information through visualization. Factors for an instructional

explanation that can promote cognitive processing of the instructional explanation (*management of processing* (Mayer, 2021)) were further regarded and implemented, e.g., through choosing case comparison as task format to promote active learning (Graulich and Schween, 2018) (Chapter 2.1.6 and 2.1.7). To illustrate how the instructional mechanistic explanations in the videos were structured and what evidence was used, Table 2 (p. 41ff.) shows an example script of the nucleophile video.

The core of the videos were *reasoning steps*, i.e., *I) inferring structural properties*, *II) verbalizing the influence on the reaction process*, *III) comparing and weighing structural properties*, *IV) making a claim based on structural properties*, and *V) linking a structural claim to energetics*. These *reasoning steps* correspond to *key aspects* of mechanistic reasoning in chemistry and regard students' explanatory approaches to solving mechanistic tasks, which are described in Chapter 2.1.2.

In the *reasoning steps*, with regard to the explicit structural difference shown in the case comparison tasks of the videos, different structural properties are inferred as causes (reasoning step I): electronegativity and delocalization in the leaving group video; hyperconjugation, inductive effects and electronegativity in the substrate video; and electron shielding/polarizability and hydrogen-bonding capabilities (capacities to form hydrogen bonds) in the nucleophile video. The structural properties are described with the effect, i.e., their influence on the reaction process (reasoning step II). Therefore, a process-oriented description of electron movement is used and a complete cause-effect rationale is established. In the further reasoning steps it is explained how the structural properties and their influence are used when comparing and weighing structural properties (reasoning step III) and making a claim based on the properties (reasoning step IV). In the last part, the task objective is restated, i.e., to decide which of the two reactions proceeds faster by determining which reaction/reaction step requires less activation energy. Thereby, the structural considerations are linked to energetics when regarding the energetic lowering of the transition state (reasoning step V).

The structure of the explanations was kept the same across the three developed videos to increase coherence.

Table 2: Structure of the developed instructional mechanistic explanation, including theoretical and empirical evidence and rationale for implementation.

Structuring element	Parts of the instructional mechanistic explanation from the nucleophile video	Evidence from…	Reasons to implement into the instructional mechanistic explanation
Description of the reactions	*In each of the reactions shown, a second order nucleophilic substitution occurs. In reaction A, a sulfur nucleophile attacks an electrophilic carbon center. In reaction B, an oxygen nucleophile attacks an electrophilic carbon center. At the same time, a chloride ion leaves the molecules. In reaction A, a thioether and in reaction B an ether are formed as products together with a negatively charged chloride ion. Both reactions proceed via a pentacoordinated transition state.*	Analysis of instructors' mechanistic explanations: use of explanatory element "description of the process" (Chapter 5.2.3)	Structuring of the explanation: including how and where to infer implicit properties from the explicit features (Chapter 5.2.3)
		Review of Chemistry Education Research findings (Chapter 2.1.2., 2.1.3)	Support cause-effect-reasoning: identifying explicit structural features, regarding dynamic changes (process-orientation) (Darden, 2002; Caspari *et al.*, 2018)
Objective	*We now have to decide which of the two reactions occurs faster. Reactions with a lower activation energy reach the transition state faster and thus have a higher reaction rate.*	Analysis of instructors' mechanistic explanations: use of explanatory element "approach" (Chapter 5.2.3)	Verbalizing the problem-solving approach with direct addressing (Chapter 5.2.3)
		Considerations of Instructional Research/ Educational Psychology Perspective (Chapter 2.1.4,2.1.5)	Means for adaptation on the language level/personalization (Kulgemeyer, 2019)
Similarities and differences	*In order to make a decision, we have to compare the similarities and differences of the two reactions.* *In both reactants, the ethyl-backbone and the leaving group, the chloride ion, are similar.* *The only structural difference between the reactions is the nucleophile. In reaction A, a negatively charged methanethiolate ion attacks the electrophilic center, while in reaction B, a negatively charged methoxide ion attacks the electrophilic center. The solvent ethanol is also similar in both cases but is able to interact with the nucleophiles in different ways.*	Analysis of instructors' mechanistic explanations: use of explanatory element "description of the process" (Chapter 3.2.3)	Structuring of the explanation: including how and where to infer implicit properties from the explicit features
		Considerations of Instructional Research/ Educational Psychology Perspective	Fostering generative processing using direct addressing (Chapter 2.1.4,2.1.5,2.1.6)
		Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)	Regarding dynamic changes with electron movement and change of electronic structure (process-orientation) (Darden, 2002; Caspari *et al.*, 2018), Support cause-effect-reasoning: identifying explicit structural features
Reference to reaction rate: **bond formation and bond breaking**	*In S_N2 reactions, the reaction rate depends on two factors, the breaking of the bond between the carbon center and the leaving group and the bond formation between the nucleophile and the electrophilic carbon atom. Since the leaving groups are identical in both cases, they influence the reaction likewise. Therefore, we only consider the bond formation between the nucleophile and the electrophilic carbon atom. This bond formation depends on how well the nucleophilic attack on the electrophilic carbon center can take place.*	Analysis of instructors' mechanistic explanations: use of explanatory element "general statement" (Chapter 5.2.3)	Structuring of the explanation: focusing on generalizable implicit-electronic relations (Chapter 5.2.3)
		Considerations of Instructional Research/ Educational Psychology Perspective	Means for structuring with the use of "rule-example"- strategy (Seidel *et al.*, 2013)
		Analysis of instructors' mechanistic explanations: use of explanatory element "approach" (Chapter 5.2.3)	Structuring of the explanation: including how and where to infer implicit properties from the explicit features (Chapter 5.2.3.)
		Considerations of Instructional Research/ Educational Psychology Perspective (Chapter 2.1.4,2.1.5,2.1.6)	Means for cognitive activation through prompts (Kulgemeyer, 2019)

Reasoning steps	Parts of the instructional mechanistic explanation from the nucleophile video	Evidence from…	Reasons to implement into the instructional mechanistic explanation:
I) Inferring of structural properties: electron shielding/polarizability & II) Verbalizing the influence on the reaction process	*As known from the periodic table, sulfur is listed underneath oxygen. Accordingly, the nucleophile with sulfur has more electrons than oxygen. Due to the larger size of the sulfur atom, the valence electrons are shielded from the nuclear charge and thus are less attracted to the charge of the nucleus. That's why they are able to move to an electrophilic center more easily.*	Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)	Support cause-effect-reasoning: using explicit structural features of the entities to infer implicit properties with their effect on the course of the reaction (e.g., Caspari *et al.*, 2018)
		Analysis of instructors' mechanistic explanations: rationale (Chapter 8) use of explanatory element "general statement" (Chapter 5.2.3)	Support cause-effect-reasoning: through the formation of complete rationales in which structural causes and associated effects are verbalized (Chapter 5.2.1, 5.2.2) Structuring of the explanation: focusing on generalizable implicit-electronic relations (Chapter 5.2.3)
	The oxygen atom in reaction B is smaller, resulting in a higher attraction of valence electrons to the charge of the nucleus. For this reason, the donation of the oxygen's electrons to form a bond is more difficult. The sulfur atom in reaction A is therefore easier to polarize compared to the oxygen atom in reaction B, and the nucleophilic attack in A is favored.	Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)	Support cause-effect-reasoning: using explicit structural features of the entities to infer implicit properties with their effect on the course of the reaction (e.g., Caspari*, et al.*, 2018)
		Analysis of instructors' mechanistic explanations: rationale (Chapter 8), use of explanatory element "general statement" (Chapter 5.2.3), use of multiple cause-effect rationales (Chapter 5.2.2)	Instead of a pure qualitative statement: implementation of the effect on structural change (to fill in the reported missing link between the structural cause and the claim about energy) (Chapter 5.2.1., 5.2.2) Structuring of the explanation: focusing on generalizable implicit-electronic properties (Chapter 5.2.3) Establishing multiple conceptual approaches considering (the change of) the electronic structure (Chapter 5.2.2)

<table>
<tr><td rowspan="2">I) Inferring of structural property: capacity to form hydrogen bonds
&
II) Verbalizing the influence on the reaction process</td><td rowspan="2">Finally, the influence of the protic solvent ethanol should be considered. In both cases an interaction between the solvent molecules and the nucleophile takes place. This interaction in form of hydrogen bonds is stronger for the less polarizable oxygen nucleophile as for the sulfur nucleophile. The oxygen nucleophile is therefore better shielded than the sulfur nucleophile. Accordingly, the nucleophilic attack occurs better with the sulfur nucleophile than with the oxygen nucleophile.</td><td>Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)</td><td>Support cause-effect-reasoning: using explicit structural features of the entities to infer implicit properties with their effect on the course of the reaction (e.g., Caspari, et al., 2018)</td></tr>
<tr><td>Analysis of instructors’ mechanistic explanations: rationale (Chapter 2.1.2, 2.1.3),

use of explanatory element “general statement” (Chapter 5.2.3)</td><td>Support cause-effect-reasoning: through the formation of complete rationales in which structural causes and associated effects are verbalized (Chapter 5.2.1, 5.2.2)

Structuring of the explanation: focusing on generalizable implicit-electronic properties (Chapter 5.2.3)</td></tr>
<tr><td rowspan="2">III) Comparing and weighing of structural properties</td><td rowspan="2">The solvent only has a minor influence in reaction A. Furthermore, the increased polarizability of the sulfur nucleophile compared to the oxygen nucleophile supports the nucleophilic attack and thus facilitates the bond formation between the nucleophile and the electrophile.</td><td>Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)</td><td>Support multivariate reasoning identification and weighing of the entities, their properties and their interplay (Kraft et al., 2010)</td></tr>
<tr><td>Analysis of instructors’ mechanistic explanations use of multiple cause-effect rationales (Chapter 5.2.2)</td><td>Establishing multiple conceptual approaches considering (the change of) the electronic structure (Chapter 5.2.2)</td></tr>
<tr><td>IV) Making a claim based on a structural property/several properties</td><td>So, the sulfur nucleophile can be considered the better nucleophile.</td><td>Review of Chemistry Education Research findings (Chapter 2.1.2, 2.1.3)</td><td>Support cause-effect-reasoning: making a claim based on properties instead of, e.g., explicit features or unproductive heuristic (Chapter 2.1.2, 2.1.3)</td></tr>
<tr><td rowspan="2">V) Linking structural claim to energetics</td><td rowspan="2">The transition state in reaction A is energetically lowered due to the supportive effects in comparison to the transition state in reaction B.</td><td>Considerations of Philosophy of Organic Chemistry (Chapter 2.1.1)</td><td rowspan="2">Support cause-effect-reasoning: connecting structural consideration with energetic considerations according to the task prompt (Goodwin, 2003)</td></tr>
<tr><td>Analysis of instructors’ mechanistic explanations: rationale (Chapter 5.2.1,5.2.2)</td></tr>
<tr><td>Final decision</td><td>That’s why reaction A occurs faster.</td><td></td><td></td></tr>
</table>

On the visual side of the tutorial videos, two reactions were displayed on a white background in the case comparisons to direct learners' attention and reduce extraneous processing (compare Figure 6, p. 24), while minimizing other distractions such as additional text or background color (*coherence principle*, *redundancy principle*). Highlighting was used to link verbal explanations to the corresponding representations (*signaling principle*). Direct addressing was used to encourage generative processing. For details on the implementation of the design principles, see Bernholt *et al.* (2023). The full-length videos are available in German (original) and English (translation) at https://osf.io/r4sx3/.

In line with the research objectives and the second assumption of this dissertation, that the qualitative analysis of students' mechanistic explanations before and after watching tutorial videos provides new insights into how to effectively construct instructional mechanistic explanations for Organic Chemistry, the main findings of study 2 are presented in the following. The findings are part of the paper presented in Chapter 9.

5.3.2. How Are Students Engaged in Reasoning Steps Before and After Watching the Purposefully Designed Videos with Instructional Mechanistic Explanations?

The qualitative analysis revealed possible effects and a lack of effects of the tutorial videos in terms of changes in students' mechanistic explanations. The results show that after watching the videos, students were able to infer more structural properties and often used them in further *reasoning steps*, e.g., comparing and weighing of several structural properties, to explain a mechanistic task.

Reasoning Step I & II:

Findings revealed that the inference of structural properties increased from before to after watching the videos (Figure 11). Further, the influence of a structural property on the reaction process (effect) was comparably often considered in the pre- and post-interviews, (Figure 11, outer ring, raspberry color; pre: 14 out of 18 properties and post: 18 out of 25 properties were verbalized with an explicit description of the influence on the reaction process).

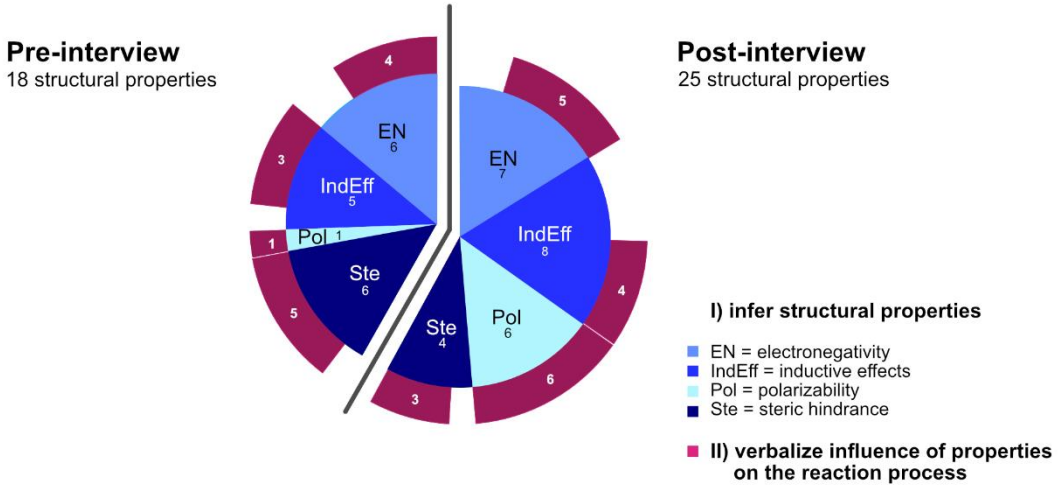

Figure 11: Pie chart representing the results of inferred properties in the pre-interview (left) and in the post-interview (right). The inner ring shows the distribution of the mentioned structural properties (shades of blue). The outer ring (raspberry colored) shows by its width how often the influence of a property of the inner ring was verbalized on the reaction process. [Reprinted with permission from [Eckhard, Rodemer, Bernholt and Graulich (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning *J. Chem. Educ*. 2022, 99, 6, p. 2236 https://doi.org/10.1021/acs.jchemed.2c00076] Copyright © 2022. Published by American Chemical Society and Division of Chemical Education, Inc.]

In particular, the structural properties not mentioned in the pre-interviews but inferred in the post-interviews were often related to the reaction process. This suggests that the newly inferred concepts were not just mentioned as “empty envelopes”, but were also verbalized in a process-oriented manner. It also suggests that students constructed meaning from the information given in the instructional explanation. Isaac’s statements from the pre- and post-interviews illustrate these findings (Figure 12).

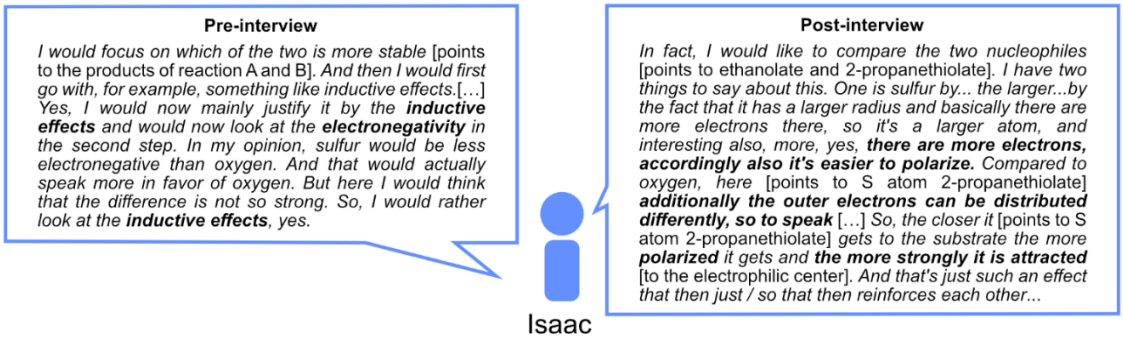

Figure 12: Isaac's statements of the pre- and post-interviews representing how he inferred structural properties (reasoning step I + II). [Reprinted with permission from [Eckhard, Rodemer, Bernholt and Graulich (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning *J. Chem. Educ*. 2022, 99, 6, p. 2237 https://doi.org/10.1021/acs.jchemed.2c00076] Copyright © 2022. Published by American Chemical Society and Division of Chemical Education, Inc.]

The quote of the pre-interview (Figure 12, left) shows that Isaac inferred inductive effects and electronegativity as causes. He relied mainly on the inductive effects of the alkyl backbone, in addition to the differing electronegativity of sulfur and oxygen. He did not

refer to nucleophilic capacities and the course of the reaction, as his focus was on determining the stability of the products to decide about a faster reaction in the pre-interview. In the post-interview (Figure 12, right), he inferred an additional structural property as he referred to the different sizes of the heteroatoms and deduced that this leads to differences in polarizability, which leads to an increased attraction of the sulfur nucleophile to the electrophilic center. Thus, after watching the videos, Isaac added an additional property to his former explanation that he related to the reaction process. He further added a reference to the electronic structure ("*the outer electrons can be distributed differently*"). As demonstrated by Isaac's explanation, students were often able to infer more structural properties after watching the videos. A participant stated within this regard ("…*it was explained in the video in such a way*." - Emil in the post-interview). Students further often verbalized the influence on the reaction process and made less use of entity-oriented approaches to determine which nucleophile is "*more stable*". Moreover, verbalization of the change provided more references to the electronic structure and electron movement after watching the videos (as can be seen in Isaacs' explanation in the post-interview).

Further, students did not tend to verbalize the influence on the reaction process (effect) for each of the mentioned properties individually. This was particularly evident in the post-interview explanations, when the students were able to derive more than one property. These findings might relate to explanations students received in instruction before, as findings on the instructors' explanations (Chapter 5.2.2), for example, showed verbalizing complete causal relationships was often neglected (almost a third of the rationales in the teaching frame did not entail effects, i.e., descriptions on how properties influence the course of a reaction). Moreover, considering multiple variables, as described in recent frameworks for mechanistic reasoning in chemistry (Chapter 2.1.2), is one of the more complex forms of problem-solving (e.g., Sevian and Talanquer, 2014), that students may not have been able to use after being "exposed" to the developed tutorial videos once. Thus, the consideration of multiple variables and their influence on the reaction process can be seen as an increasing cognitive demand that not all of the students were able to cope with (Sweller, 1988; Chi, 2006).

Overall, the findings indicate that the instructional mechanistic explanation was often perceived as relevant by the students and was able to tie in with the students' prior knowledge, which has been suggested to be valuable for learning from an instructional perspective (Wittwer and Renkl, 2008).

Reasoning steps III; IV; V:

In addition, it was of interest how the students were engaged in further *reasoning steps* during the problem-solving process before and after watching the videos (Figure 13). As shown in Figure 13, the use of reasoning steps *III) comparing and weighing structural properties* and *IV) making a claim based on structural properties* increased, whereas reasoning step *V) linking a structural claim to energetics* was not mentioned before and after watching the videos; hence, no change could be observed.

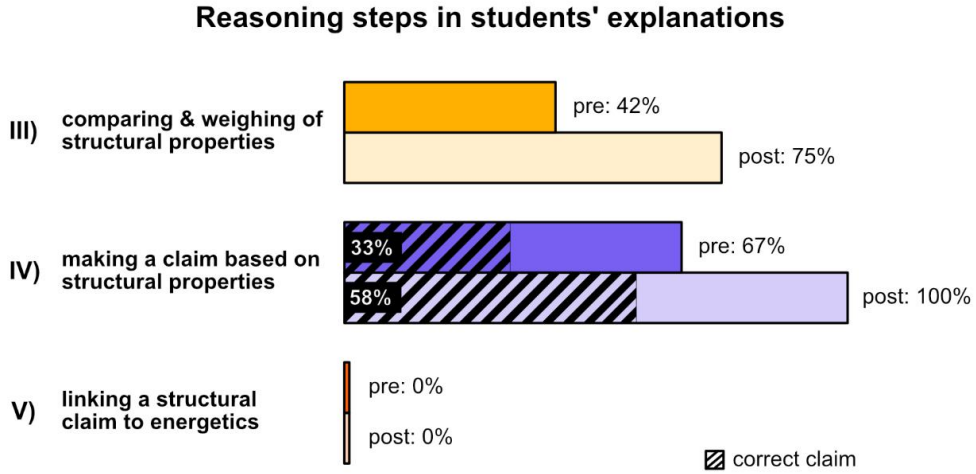

Figure 13: Reasoning steps in students' (N =12) explanations before (pre) and after (post) watching the videos. Yellow bars: reasoning step *III) comparing & weighing structural properties*. Purple bars: reasoning step *IV) making a claim based on a structural property/several structural properties* (before watching the videos a third of the students did not make a claim, another third stated correct claims (indicated by the shaded areas), whereas the other third stated incorrect claims; in the post-interview: 58% of the claims were correct (indicated by the shaded areas). Orange bars: reasoning step *V) linking a structural claim to energetics*. [Reprinted with permission from [Eckhard, Rodemer, Bernholt and Graulich (2022). What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning *J. Chem. Educ*. 2022, 99, 6, p. 2238 https://doi.org/10.1021/acs.jchemed.2c00076] Copyright © 2022. Published by American Chemical Society and Division of Chemical Education, Inc.]

The increase in comparing and weighing multiple structural properties (reasoning step III) indicates that the tutorial videos, i.e., the instructional mechanistic explanations, can support students in multivariate thinking (in short-term). Findings also point to students having difficulty deciding which of the properties influencing the reaction process is dominant. Determining the relative strength of influences, such as whether inductive effects outweigh potential steric hindrance, for example, appears challenging for students. Again, this may be because students were only exposed to the instructional explanation in the tutorial videos once (i.e., reflecting a lack of acquired conceptual understanding), or it may be due to what students are accustomed to perceiving as instructional mechanistic explanation. Regarding the latter, some of the instructors' explanations of the first study showed that a final claim for a task was often formed by stating qualitative differences without referring to the source of this qualitative difference, i.e., weighing and comparing

the influences of a structural property on the course of a reaction (Chapter 5.2.2). Therefore, students' challenges may also arise from the adaptation to the ways in which they are accustomed to providing explanations (e.g., stating qualitative differences without reasoned weighing).

In addition, the results showed that after being engaged with the instructional mechanistic explanation in the videos, all students made a claim based on one or more structural properties. The increase of the reasoning step *IV) making a claim based on structural properties* from pre to post (Figure 13, purple bar) underscores that students often had changed their approach to solving a case comparison, in terms of moving away from basing their claim on surface features or gut intuition. It should be noted that whereas in the pre-interviews, correct claims were often based on heuristics, such as relying on memorized reactivity orders, in the post-interview, correct claims were often made based on multiple structural properties and their weighing. This indicates that the use of *general statements* and rules in the instructional mechanistic explanations in the videos, as well as providing a problem-solving *approach* by explaining how to infer and use structural properties, might supported the students in their problem-solving in the post-interview.

Furthermore, the results show that the instructional mechanistic explanations did not have an impact on the students' connection between structural considerations and the energetics of a reaction. As demonstrated in previous research, this reasoning step was often found to be challenging for students. Students struggled to connect structural assumptions to energy, e.g., when reasoning about rate-determining steps (e.g., Taber, 2009; Becker and Cooper, 2014; Caspari *et al.*, 2018; Popova and Bretz, 2018; Bodé *et al.*, 2019). In the post-interview, students' statements indicated that they were often aware that this step was part of solving a case comparison task, but they did not verbalize this step themselves. Isaac's explanation shows why he did not include reasoning about the energetic course in his explanation: "*But the thing with the speed and the activation energy, how that is connected* […] *I am not quite aware of this causality yet.".* As his statement illustrates, it is difficult (for him) to understand "*this causality*", i.e., the connection between structural and energetic considerations. Challenges in making these connections may arise because, on the one hand, they may not have been explicitly emphasized or demonstrated enough in the designed instructional mechanistic explanation. On the other hand, students may not be accustomed to making connections between structure and energy because the energy concept is often considered prior knowledge (Becker and Cooper, 2014). Furthermore, the unfamiliarity of the task format may have played a role. In addition, the energy claims were made at the end of the video, which may have overloaded students' working memory and exceeded their attention span (Mayer, 2021).

This suggests that for students in this cohort, more explicit emphasis should have been placed on reasoning about the energetic course of the reaction. Further instructional adaptations to promote structure-energy connections might include the use of task formats that explicitly ask students to make energetic claims, or the implementation of approaches to the causality of structural and energetic considerations, or the use of additional visualizations (e.g., of the energetic course) in the instruction.

In conclusion, the instructional mechanistic explanation in the tutorial videos seems to be appropriate in highlighting the influencing factors of a nucleophilic reaction (nucleophilicity, leaving group quality, substrate effects). Differentiated content analysis revealed how students adapted different aspects of the instructional mechanistic explanation, indicating gains in conceptual and procedural knowledge after watching the videos. Students were often able to infer more structural properties and use these to make reasoned structural claims, i.e., to perform essential reasoning steps when problem-solving, moving away from reliance on surface features and memorized reactivity orders. However, after watching the videos, weighing multiple variables and relating structural considerations to the energetic course proved challenging, calling for means to adapt the instructional mechanistic explanation to the needs of the cohort.

6. Conclusions

With respect to the guiding question, this dissertation has shown how theoretical and empirical considerations from different research perspectives (Chapter 2), together with empirical findings on instructors' mechanistic explanations, provide guidance for the construction of instructional mechanistic explanations in Organic Chemistry. Through the qualitative analysis of Organic Chemistry instructors' explanations (Chapters 5.2 and 8), this dissertation added new insights of instructional practice to the construction of instructional explanations for Organic Chemistry. Instructors often considered the prior knowledge of the target group, and adapted their explanations accordingly, either in a concise way (e.g., focus on keywords in the *expert frame*) or in a more elaborate way (e.g., use of implicit features, complete and combined *cause-effect rationales* and additional *explanatory elements* in the *teaching frame*). Further, a great deal of variation in the use of cause-effect rationales in the two frames across instructors and tasks could be revealed. While some instructors decided to use more implicit information in light of the frame shift, others did not change their explanatory approaches, as they may not have seen the need to elaborate explanations for the fictional students they had in mind in the *teaching frame*. This reiterates the importance of being aware of students' prerequisites when constructing instructional explanations. Further analysis revealed the instructors' differentiated use of *explanatory elements*, i.e., *description of the process*, *general statements*, and *approach*. These elements were used differently to embed the rationales in both frames and could refer to instructors' affordances to support students' cognitive activation and knowledge construction. Therefore, based on the instructors' explanations and how *framing* changed their explanatory approaches, the following implications can be drawn for instructional settings and resources aimed at supporting students' mechanistic problem-solving:

- support cause-effect-reasoning: through the formation of complete rationales in which structural causes and associated effects are verbalized;
- stating tasks objectives by explicitly verbalizing how to make claim, i.e., the need to use implicit properties as structural causes of an effect in order to make claims about energy;
- making problem-solving approaches explicit, including how and where to infer implicit properties from the explicit features;
- when using multiple rationales, i.e., multiple conceptual approaches, interrelating links should be made in terms of considering (the change of) the electronic structure;

- when stating general statements focusing less on generalizations based on explicit differences, rather generalizable implicit-electronic properties and relations should be stated.

The research on how instructors provide mechanistic explanations in different frames is new to the field. By providing an instructional perspective, the findings contribute to the growing body of research on mechanistic reasoning in Organic Chemistry and allow for reflection on instructional influences on student mechanistic reasoning.

This dissertation further provided new insights of how instructional mechanistic explanations could be designed and implemented in tutorial videos for Organic Chemistry (Chapter 5.3).

By combining considerations from:

- Philosophy of Science (e.g., inclusion of aspects: entities, properties, interactions; claims about structure and energy),
- Instructional Research (e.g., adaptation to students' prerequisites, avoidance of digressions), and
- Multimedia Research (e.g., management of cognitive processing through implementation of design principles) **with**
- theoretical and empirical findings from Chemistry Education Research (e.g. key elements: support for the establishment of cause-effect relations), and
- findings on instructors' mechanistic explanations (e.g., support for knowledge construction through the provision of problem-solving approaches),

instructional mechanistic explanations for nucleophilic substitution reactions for tutorial videos were developed and tested (Chapter 5.3.1, Table 2, p. 41).

Overall, the implementation of instructional mechanistic explanations in tutorial videos enabled students to advance their own mechanistic explanations (Chapter 5.3 and Chapter 9) by supporting them in the inference of (multiple) structural properties and the use of properties in their problem-solving. It was found that the reasoning step of *inferring effects of (multiple) structural properties* and *weighing and comparing* them is challenging for students. The results showed that students were not supported in making a connection between structural considerations and the energetics of a reaction. Instead, students often relied on "*stability*" to determine which reaction proceeds faster. Thus, when advancing the instructional mechanistic explanations, the link between structural and energetic changes could be strengthened, e.g., using "*stability*" as a connector to bridge the "*stability of products*" to the activation energy and the reaction rate (Goodwin, 2003). It was also

shown that all students made a claim based on one or more structural properties after the intervention. This indicates that students had changed their approach, moving away from basing their claim on surface features and were supported in linking implicit information of properties and concepts to the explicit representations. Thus, the videos enhanced students' conceptual understanding. Overall, the developed instructional mechanistic explanations in the tutorial videos support students in overcoming the use of unproductive heuristics (e.g., reliance on surface features) or simple recall (e.g., order of reactivity) by providing a meaningful approach to solving mechanistic tasks of nucleophilic reactions. In addition, the instructional mechanistic explanations in the tutorial videos make the structure of an expected explanation transparent and therefore accessible to students.

As limitation, it should be noted that the instructional mechanistic explanations in the videos presuppose prerequisites of the difficulties reported as common in mechanistic problem-solving and were designed according to the course scripts and module manuals (Chapter 2.1.2). In other words, they are aimed at a broader audience and not at the needs of individual students. In addition, only the mechanism type of nucleophilic substitution reactions has been included in the videos. However, this type of mechanism represents prototypical concepts and questions about transformations that are transferable to different types of mechanisms in Organic Chemistry. Further, it remains open whether learners reverted to an illusion of understanding (Kulgemeyer *et al.*, 2022) after watching the videos and, accordingly, only referred to it in the post-interview tasks in study 2, which had similar surface features as the tasks presented in the videos. Implementing transfer tasks into the post-interviews would have been useful, as would further investigation into the extent to which the use of case comparison in videos allows for deeper processing to prevent illusion of understanding. Exploring different mechanistic contents/types of mechanisms would further increase the generalizability of the results. Further limitations and implications are presented in the papers in Chapter 8 and 9.

This dissertation contributes to filling the gap between research on the design of tutorial videos and research on the effectiveness of instructional explanations on student learning (Brame, 2016; Kulgemeyer and Peters, 2016) by showing how to construct instructional mechanistic explanations for their implementation in tutorial videos and how they influence students' problem-solving in Organic Chemistry.

Evidence-based constructing and empirically testing the effectiveness of instructional mechanistic explanations lays the groundwork for implementation in practice in Organic Chemistry. On the one hand, for instructors in the classroom, which supports instructors in their role as a lynchpins for the mediation of mechanistic reasoning, and on the other

hand, for tutorial videos for Organic Chemistry, which represents an opportunity to support students with an emerging multimedia learning resource.

6.1. Outlook and Implications for Future Implementation

The focus of this dissertation has been the development and testing of instructional mechanistic explanations in Organic Chemistry. The results provide implications for the extension and implementation of the instructional mechanistic explanation and for further research.

Developing a Scaffold for Constructing Instructional Mechanistic Explanations in Organic Chemistry

Based on the theoretical and empirical considerations from the different research directions (Chapter 2), including considerations of a recently developed framework for effective instructional explanations in Science Education (Kulgemeyer, 2019), the findings on instructors' mechanistic explanations (Chapter 5.2.), and the findings on the effectiveness of the developed instructional mechanistic explanations (Chapter 5.3.), a question-guided scaffold for the construction of effective instructional mechanistic explanations in Organic Chemistry was developed (Figure 14, p. 55).

The scaffold could serve as a guide for developing further instructional mechanistic explanations for multimedia resources and for experienced instructors to plan their instruction in detail. It could also serve as a tool for novice instructors, as studies have shown that explaining in an instructional context is a major challenge for novice instructors (Inoue, 2009; Zotos *et al.*, 2020).

The question-driven scaffold (Figure 14) places the prerequisites of the addressees at the center, as Instructional Research has shown that adapting to the prerequisites of the addressees plays a key role in the effectiveness of an instructional explanation (Wittwer and Renkl, 2008; Kattmann, 2016; Gropengießer and Marohn, 2018). Further evidence of the key role of the prerequisites of the addressees was found in the second study. Since none of the students included the *reasoning step* of *making a claim about energy* in their reasoning, it can be expected that the affordances of the implementation of the *reasoning step* did not match the students' prerequisites. In addition, the analysis of the instructors' explanations in the first study revealed ways of adapting to the prerequisites of the addressees, which is another indication of the key role. The need to adapt to specific addressees' prerequisites was mentioned by instructor Smith in an aside after the *expert frame*:

Instructor Smith: "*If you ask about the speed of the reaction, then you would have to work with the activation energies and I cannot just say 'the more stable cation is formed, therefore it reacts faster'. It depends on which level of explanation I adapt. So, in school, that is certainly how you would explain it. Um. In an introductory Organic Chemistry course, I would work with energy diagrams to correlate the transition state with the product, in this case [referring to task 1] the cation, according to the Hammond postulate for this exothermic step."*

He was aware of the need for adaptation of his short statement in the *expert fram*e to the respective addresses and mentioned means of adaptation. For example, he would include more implicit information or choose different forms of representation (e.g., energy diagrams, which could also have supported students in the cohort in study 2.) to accompany his instructional explanation for different addresses – aspects that were also included in the scaffold (Figure 14).

In order to consider the addressees' prerequisites, a diagnosis is required. For smaller groups of learners, diagnostic tasks are appropriate (for examples see: Christiansen, 2007; Barke *et al.*, 2015). For larger groups of learners, as in lectures, automated assessment tools can be used to provide feedback on the learner's prerequisites. In this regard, Yik and colleagues (2023) have developed an automated formative assessment tool in the area of Lewis acid-base mechanisms (Yik *et al.*, 2023) (and other tools for diagnosing mechanistic understanding are emerging (for a review see: Martin and Graulich, 2023)). With the automated feedback on students' current understanding combined with the considerations of the scaffold (Figure 14), instructors could customize their instructions. Yik and colleagues (2023) exemplified within regard to students' prior knowledge of understanding of Lewis acids and bases "*if the majority of the class is found to not correctly use the Lewis acid−base model, instructors may choose to dedicate some time in the next course meeting to discuss differences between the Brønsted−Lowry and Lewis models* […]" (Yik *et al.*, 2023, p. 3110). When using the scaffold (Figure 14), instructors might additionally consider the depth of their instruction. For example, they might think about ways to support cognitive activation, i.e., problem-solving *approaches* to help students identify the electron density centers to support identification of Lewis bases and acids. Alternatively, given the guiding question of the scaffold, they might consider how to construct the *reasoning steps* of the mechanistic explanation, i.e., using electronic structure and properties to distinguish the capacities of Lewis acids and bases and Brønsted acids and bases.

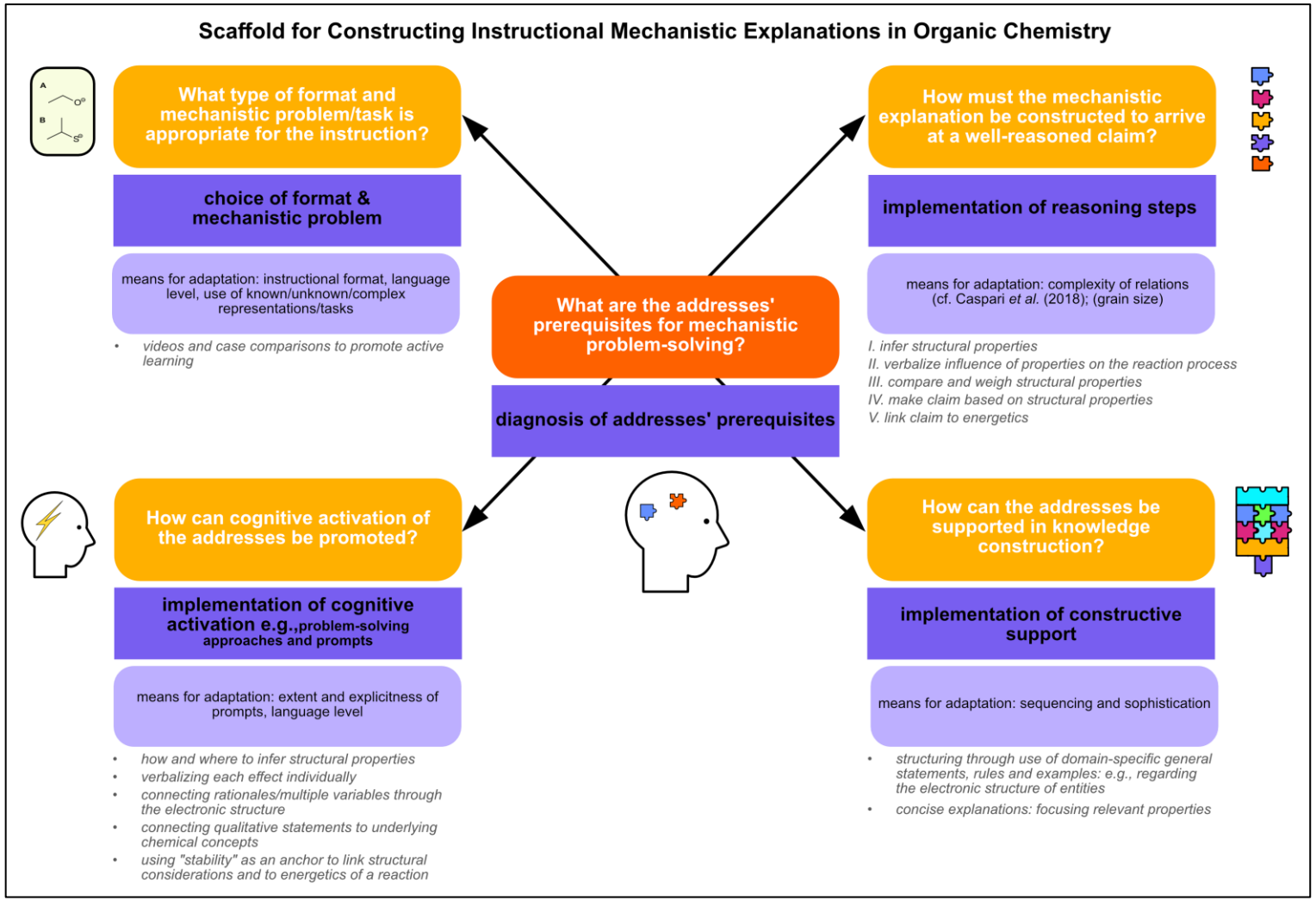

Figure 14: A scaffold for the construction of instructional mechanistic explanations in Organic Chemistry. The yellow boxes indicate guiding questions; the purple boxes indicate means for adaptation to meet addresses' prerequisites. The gray implications show how the instructional mechanistic explanation was constructed for study 2.

Hence, the scaffold in Figure 14 provides *guiding questions* (yellow boxes) that could be useful for instructors to prestructure their explanations in a targeted way. The results of the first study indicate the potential benefits of a scaffold within that regard. During the first study, the instructors often assured themselves as to how they should interpret the *teaching frame* and whether they would have time to prepare themselves to provide a didactically meaningful explanation. For example, after giving the prompt of the *teaching frame*, instructor Lewis ensured if there was time to do so.

Interviewer: "*Now we go on with your explanation [in the teaching frame]."*

Instructor Lewis: "*Okay. But I still have time to prepare for it, to explain in a didactically meaningful way?"*

Interviewer: "*Of course. But the task format is the same like before [in the expert frame]."*

Instructor Lewis: "*Okay, sure. Still, I think there [in the expert frame] I was thinking more for myself, so to speak, and not thinking about how to get there in a meaningful way."*

His statement indicates that he was thinking about changing his approach to explanation from "*thinking more for myself*" to explaining in a "*meaningful way*" within the *teaching frame*. Prior to giving his explanation in the *teaching frame* – in contrast to the *expert frame* – he took some time to prepare. Then, he intentionally designed his explanation to provide guidance on how to arrive at a reasoned claim, e.g., "*how to get there*" through process-oriented verbalizations and thoughtful *approaches*. Regarding instructor Lewis' side comment, the question-guided scaffold (Figure 14) could guide instructors to reflect on "*meaningful ways*" to customize their instructional mechanistic explanations. In addition to the guiding questions, the scaffold provides *means of adaptation* (purple boxes) that offer suggestions on how instructors can tailor their instructional mechanistic explanations to students' prerequisites, e.g., by implementing problem-solving prompts (how and where to infer properties), by adjusting the complexity of the causal relations (e.g., implicit-electronic causes with electronic effect) or the level of language they use. In order to determine the effectiveness of the scaffold, empirical studies are needed.

6.2. Implications for Future Research

Given the limitations of the studies, different research designs could be tested to verify validity. With regard to the first study, a larger study with a larger number of instructors as well as a different mechanistic task could be conducted. Since the *framing construct* was used in study 1, a further study could explore teaching-learning situations in which the

instructor and the students are engaged on-the-spot and in which the instructors can adapt their explanations in a more authentic way to the specific students.

With regard to the second study, additional instructional mechanistic explanations (and tutorial videos) could be designed using the scaffold (Figure 14) to more specifically address individual needs. In a digital learning environment, specifically designing instructional mechanistic explanations could be achieved through automation by combining “modular explanatory elements” that were diagnosed as challenging for an individual learner. As the results of the second study revealed difficulties in the verbalization of some of the *reasoning steps*, implementing these with an approach on how to do so, might foster students’ understanding (e.g., approach on how to link structural considerations with energetic considerations).

A further study could consider variations in intrinsic load (in addition to the possibility of varying extrinsic load through different types of highlighting), i.e., varying the difficulty of the tasks or the complexity of the language presented during instruction. Another aspect concerns working memory capacity. Students did not link structural to energetic accounts in the post-interviews. This might be due to the fact that the reference of linking structural and energetic accounts was made at the end of the video. It can be argued that students’ working memory capacity was exceeded at the end of the videos, resulting in a decrease of attention. Hence, one might emphasize the *reasoning step* of linking structural to energetic considerations at the beginning of an instructional explanation to support cognitive processing and prevent attentional overload at the end.

Future studies could regard individual prior knowledge. From the findings, it remains to be seen whether students with high prior knowledge will be more likely to adapt the *reasoning steps* and be able to use them in new contexts after being engaged with the instructional mechanistic explanation in the videos, whereas students with low prior knowledge might be more likely to focus on the declarative information conveyed in the videos, e.g., be able to repeat key terms of chemical concepts. In this regard, Kulgemeyer (2020) reported that instructional videos may primarily promote declarative knowledge, while transferable, conceptual knowledge benefits from additional instruction, i.e., the use of learning tasks that require application of the principles explained in the videos to new contexts to promote active learning. Thus, the impact of different instructional mechanistic explanations on students’ problem-solving could be further investigated, with a focus on the prior knowledge and the embedding of the explanation in the instruction (for example, with or without a learning task).

Next to long-term effect on learning, further research could also address the quality of the constructed instructional mechanistic explanations in Organic Chemistry in more detail, for example through exploring the effects of sequencing or the implementation of specific *explanatory elements* (e.g., problem-solving approaches). A challenge, however, is controlling for potentially confounding variables to test the effectiveness of each developed explanation. This implies developing an evidence-based framework, based on the construction of instructional mechanistic explanations and findings (Chapter 5), that provides more information about the efficacy of instructional mechanistic explanations for student learning *in Organic Chemistry*.

This dissertation has demonstrated the construction of an instructional mechanistic explanation in Organic Chemistry by combining theoretical and empirical findings from multiple disciplines (Chapter 2) with insights from instructors' (instructional) explanations (Chapter 5.2). The instructional mechanistic explanation was implemented in tutorial videos to test whether it could support student mechanistic problem-solving. Qualitative content analysis revealed learning gains from watching the tutorial videos by showing that the modeled *reasoning steps* of the developed instructional explanation were evident in students' explanations and that students based their claims on structural properties rather than explicit features or memorized reactivity orders (Chapter 5.3). Overall, the findings of this dissertation within the EYE-OC project suggest that the developed tutorial videos with the implemented instructional mechanistic explanations are a possible approach to support students' mechanistic problem-solving. These findings will not only inform teaching and learning in Organic Chemistry, but will also serve as a basis for developing instructional materials that combine instructional mechanistic explanations with emerging multimedia formats.

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8. Let’s Frame it Differently – Analysis of Instructors’ Mechanistic Explanations

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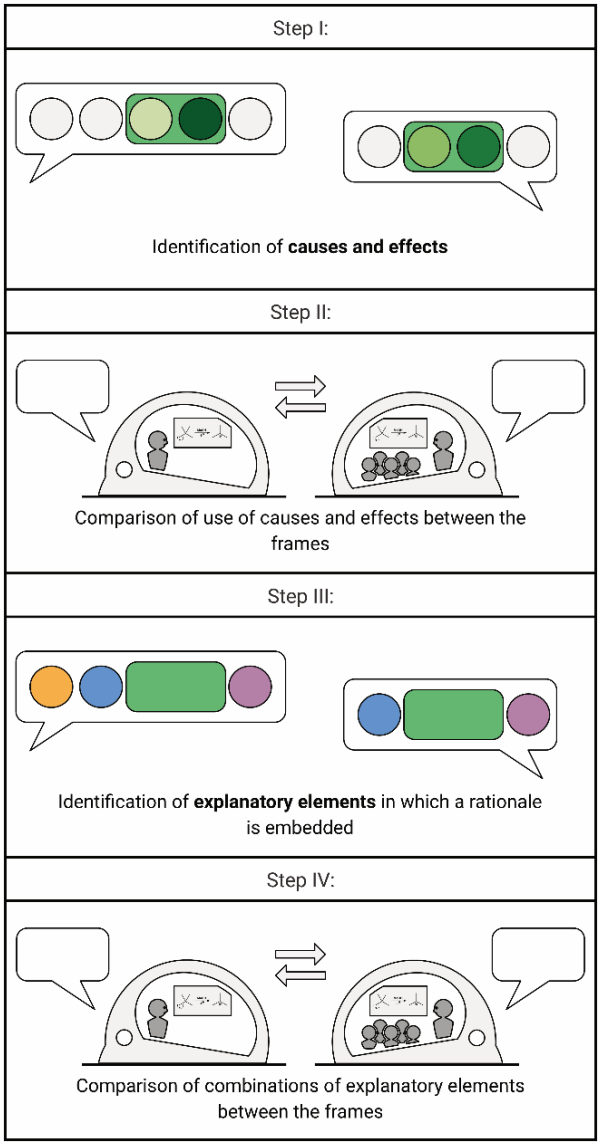

Figure 15: Overview of Data Analysis. Reproduced from (Eckhard *et al.*, 2022, p. 83) with permission from the Royal Society of Chemistry.

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Let's frame it differently – analysis of instructors' mechanistic explanations

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Research in Organic Chemistry education has revealed students' challenges in mechanistic reasoning. When solving mechanistic tasks, students tend to focus on explicit surface features, apply fragmented conceptual knowledge, rely on rote-memorization and, hence, often struggle to build well-grounded causal explanations. When taking a resource perspective as a lens, students' difficulties may arise from either an unproductive or a missing activation of cognitive resources. Instructors' explanations and their guidance in teaching situations could serve as a lynchpin to activate these resources. Compared to students' challenges in building mechanistic explanations in Organic Chemistry, little is known about instructors' explanations when solving mechanistic tasks and how they shape their targeted explanations for students in terms of the construction and embedding of cause–effect rationales. This qualitative study aims to contribute to the growing research on mechanistic reasoning by exploring instructors' explanatory approaches. Therefore, we made use of the framing construct, intended to trigger certain frames with explicit instruction. Ten Organic Chemistry instructors (university professors and lecturers) were asked to solve case comparison tasks while being prompted in two scenarios: an expert frame and a teaching frame. Our analysis shows that there is a shift from instructors' mechanistic explanations in the expert frame towards more elaborated explanations in the teaching frame. In the teaching frame, contrary to what might be expected, complete cause–effect relationships were not always established and instructors differed in how they shaped their explanations. Additional explanatory elements were identified in both frames and their shift in use is discussed. Comparing approaches between frames sheds light on how instructors communicate mechanistic explanations and allows us to derive implications for teaching Organic Chemistry.

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Introduction

In a time of global challenges, conspiracy theories, and fake news, the ability to construct well-grounded explanations can be regarded as a necessary skill. The importance of constructing explanations is not only evident in the growing body of literature in which the nature and types of explanations (Hempel, 1965; Achinstein, 1983; Salmon, 1984) and the structure of explanations and arguments (Toulmin, 2003) are discussed, but also in recent science curricula. The construction of scientific explanations promotes the understanding of ideas and claims made in science (*e.g.*, Driver *et al.*, 2000; Duschl and Osborne, 2002).

When considering scientific explanations, mechanistic explanations are of interest as they entail the prediction and explanation of phenomena (Machamer *et al.*, 2000; Craver and Darden, 2013). Building mechanistic explanations requires accounting for how and why a phenomenon comes about, and consideration of the interaction of factors leading to a specific phenomenon (Machamer *et al.*, 2000). The entities of a mechanism with their properties, activities, and specific organization (temporal and spatial) need to be regarded (Machamer *et al.*, 2000; Craver and Darden, 2013), and integration and shifting between levels is often required, *i.e.*, different granularities in a description – macroscopic, submicroscopic or symbolic – must be considered (Gilbert and Treagust, 2009; Krist *et al.*, 2019).

Focusing on students' mechanistic explanations in the context of Organic Chemistry reveals that students often rely on explicit instead of implicit features (Bhattacharyya and Bodner, 2005; Strickland *et al.*, 2010; Anzovino and Bretz, 2016; Graulich and Bhattacharyya, 2017). They are known to use simplified pattern recognition, rote-memorization, and heuristics (Maeyer and Talanquer, 2013; Graulich and Bhattacharyya, 2017; Galloway *et al.*, 2019). These strategies often result in

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unsuccessful solutions and hinder meaningful learning. Hence, difficulties in mechanistic reasoning can be attributed to challenges in appropriately inferring implicit information and building causal relationships.

Recent studies of students constructing mechanistic explanations further underline the fact that they often struggle to make claims acknowledging causal relationships. Moreira *et al.* (2019a), for instance, revealed that fewer than half of the students in their study generated causal explanations; they typically relied on re-describing entities and properties without attempts to build causal links between them. Similar observations were made by Weinrich and Talanquer (2016), who found that students often relied on descriptive and relational accounts by considering properties or activities without associating them in a causal manner and without describing phenomena "[. . .] as sequential chains of events with causes and effects" (Weinrich and Talanquer, 2016, p. 400), which would correspond to a linear causal account.

As findings of prior research underline, the ability to build causal relationships can be regarded as crucial to explain, predict, and understand mechanistic processes. Accordingly, there is a need to promote the understanding of causality in teaching mechanisms. As instructors influence how students approach problems, and reason while constructing scientific explanations (*e.g.*, Russ, 2018; Moreira *et al.*, 2019b), the role of instructors as lynchpins has to be acknowledged. In this regard, little is known about instructors' approaches when solving and explaining mechanistic problems and how they shape their explanations when targeting explanations for students. On the one hand, it is assumed that instructors, as experts in their domain, have great and varied content knowledge, which is organized in high-order knowledge structures. This enables them to activate resources in a way that reflects the task demands (diSessa and Sherin, 1998; Talanquer, 2018a). On the other hand, instructors, as teachers, are expected to possess pedagogical content knowledge (Shulman, 1986). They are required to appropriately transform knowledge of a domain for the teaching context.

Instructors as a lynchpin for constructing mechanistic explanations

The influence that instructors and teachers have on student learning and achievement is widely recognized (Hattie, 2008). Instructors' impact on the development of students' reasoning skills has been increasingly appreciated over recent years, *e.g.*, with regard to teachers' instructional strategies such as making the rationale of scientific explanations explicit or defining scientific explanation (*e.g.*, Osborne *et al.*, 2004; McNeill and Krajcik, 2008).

The influence instructors have on students' ability to construct and apply mechanistic explanations is highlighted in chemistry education as well. Talanquer (2018b), for example, stated "Chemistry instructors at all educational levels should foster students' ability to spontaneously and productively apply chemical mechanisms in their sense-making and meaning-making activities regardless of the context" (Talanquer, 2018b, p. 1906).

Instructors do not only play a crucial role on what and how is being learned but how to assess learners' abilities. As Stowe and Cooper (2019) state "[. . .] assessments should not simply ask for recall of facts but rather for use or knowledge to predict, explain, and/or model phenomena." (Stowe and Cooper, 2019, p. 601).

An instructor's teaching of mechanisms and the influence on students' reasoning was recently analyzed by Moreira and colleagues (2019b). In their study, teacher–student-interactions as well as modes of reasoning (Sevian and Talanquer, 2014) used by the students and the instructor were analyzed. In the observed lesson, the instructor emphasized simple causal explanations. After the lesson, a trend towards students constructing simple causal explanations from both directions (*i.e.*, from both more simplistic modes of reasoning and more sophisticated modes of reasoning towards simple causal explanations) was observed. Hence, the instructor's modes of reasoning, *i.e.*, her explanations, influenced students' expressed reasoning (Moreira *et al.*, 2019b). Therefore, the instructor can be regarded as a lynchpin for the construction of students' mechanistic explanations.

As instructors are one of the key factors when learning Organic Chemistry at the university level, it is important to investigate how they verbalize and transform their content knowledge of mechanisms into mechanistic explanations in a teaching context, compared to their more typical professional context as domain experts. We use the framing construct, which acknowledges that a certain frame (*i.e.*, interpretation of a situation) triggers particular behavior (Goffman, 1974; Tannen, 1993; MacLachlan and Reid, 1994), to explore how instructors make use of causes and effects when explaining mechanistic tasks in different frames, and how they combine their cause–effect rationales with further explanatory elements. By elucidating instructors' mechanistic explanations, we aim to infer implications for teaching to promote causal accounts in mechanistic reasoning.

Theoretical framework

Causality as a core element of mechanistic reasoning

To characterize mechanistic reasoning in chemistry contexts, several authors suggested frameworks to analyze students' explanations (*e.g.*, Sevian and Talanquer, 2014; Becker *et al.*, 2016; Cooper *et al.*, 2016; Caspari *et al.*, 2018). These frameworks offer valuable approaches to conceptualize mechanistic reasoning through consideration of mechanistic aspects such as explicit and implicit properties, statics and dynamics in a mechanism, consideration of cause–effect relations, and weighing of multiple variables. Commonalities are evident, such as that arguments or mechanistic explanations categorized at the most elaborated level go beyond a pure description of a mechanism, capture the idea of process-orientation, and include aspects of causality. The latter can be considered one of the core elements of mechanistic reasoning. Early approaches that characterize causality in mechanistic reasoning describe a causal mechanism as an explanation of "the process by which a cause brings about an effect" (Koslowski, 1996, p. 13). This is in line with the assumption of Russ *et al.* (2009) who claim that reasoning about causality itself through identifying causal factors is not sufficient

to generate mechanistic explanations. The "*how* 'X' brings about 'Y'" (Russ *et al.*, 2009, p. 881) needs to be considered together with the process regarding the interacting causal factors, which requires the consideration of causes and effects.

Although frameworks analyzing mechanistic reasoning in chemistry contexts include causality as a major focus, they have different approaches to complexity or elaborateness in students' responses. Sevian and Talanquer (2014) developed a framework that considers four modes of reasoning, in which causal aspects are described in the higher reasoning modes, *e.g.*, in the linear causal mode by inferring explicit and implicit properties, identifying organization, connections and interactions between entities, and building linear cause–effect relations (Sevian and Talanquer, 2014). Cooper and colleagues differentiate between the causal and mechanistic part of a causal mechanistic explanation (Becker *et al.*, 2016; Cooper *et al.*, 2016; Crandell *et al.*, 2018). Their causal-mechanistic-reasoning framework allows to analyze whether students take into account *what* is happening, *how* it is happening, and *why* it is happening, by categorizing students' utterances into descriptive (what), mechanistic (what and how), causal (what and why), and causal mechanistic answers (what, how, and why) (Cooper *et al.*, 2016; Crandell *et al.*, 2018). Becker *et al.* (2016) further analyzed student explanations in various dimensions: non-canonical or canonical, and non-electrostatic or electrostatic. They consider if an explanation includes references to the underlying mechanism (Becker *et al.*, 2016). The framework developed by Caspari and colleagues (2018) characterized the structure of comparative mechanistic reasoning with different levels of complexity of cause–effect relations (Caspari *et al.*, 2018).

Besides different approaches to complexity or elaborateness in students' responses, the frameworks also differ in the graduations of causality in their coding schemes: they differ in how specific the description of causes and effects in student responses should be, and which grain size the explanation requires to be causal. In comparative mechanistic reasoning (Caspari *et al.*, 2018), for an explanation to be considered causal a cause and an effect must always be verbalized on an electronic level. The causal-mechanistic-reasoning framework (Cooper *et al.*, 2016) requires reasoning to be explained one scalar level below the phenomenon, whereas in the modes of reasoning the granularity of a causal answer is not defined. Hence, a causal answer could entail a cause–effect relation at varying levels of granularity, *e.g.*, including reasoning about explicit structural features or implicit concepts (Sevian and Talanquer, 2014; Bodé *et al.*, 2019).

Although the frameworks that characterize mechanistic reasoning in chemistry contexts seem to differ, they all consider causality of explanations as some answer to "the why" question, entailing a description of causal factors and their effects. Hence, based on the notion of causality, causes and effects can be regarded as a core element of mechanistic explanation.

Framing as a lens to elicit variations in resource activation

The *resource-based framework* (Hammer *et al.*, 2005) defines knowledge and the ability to reason about something "as comprised of many fine-grained resources that may be activated or not in any particular context" (Hammer *et al.*, 2005, p. 92). This context-dependency of resource activation can be attributed to individuals having different expectations of how to (inter) act (Tannen, 1993). To ascertain one's own expectations, one answers the question "What is it that's going on here?" (Goffman, 1974, p. 8) to *frame* a situation (Goffman, 1974; Tannen, 1993; MacLachlan and Reid, 1994). Hutchison and Hammer (2010) stated that "[…] framing shapes how people experience the situation, form expectations, and make choices" (Hutchison and Hammer, 2010, p. 509). Accordingly, an individual's framing of a context determines their resource activation and can thereby influence the engagement in situations differently. Hammer *et al.* (2005) exemplified this by noting that "[a] student may frame a physics problem as an opportunity for sense making, or an occasion for rote use of formulas" (Hammer *et al.*, 2005, p. 98). Thus, the engagement in constructing explanations can be attributed to different framings of the instruction. In chemistry contexts, framing has been used to investigate students' argumentative discourse in a laboratory activity in terms of triggering a certain frame with explicit instruction, *e.g.*, by explicit deployment of task operators (*predict-verify frame vs. observe-infer frame*) (Petritis *et al.*, 2020). Results showed that framing affects the engagement in argumentation as well as the sophistication and completeness of arguments, *e.g.*, in terms of which chemical concepts were used and if connections were made between evidence and claims (Petritis *et al.*, 2020). The induction of different frames due to different contextual features in prompts was further realized by Slominski *et al.* (2020) to analyze researchers' or instructors' (*i.e.*, experts from biology, physics, and engineering departments) reasoning approaches (Slominski *et al.*, 2020).

In summary, one can state that individuals' approaches or activation of resources in a situation depend on individuals' framing of a situation, which is influenced by experience but also by explicit instruction (*i.e.*, prompting). Comparing explanations of two differently framed prompts allows the effect of each prompt to be elicited and changes made when shifting from one frame to the other. Therefore, in this study we made use of framing to elicit instructors' variations of explanatory approaches when solving mechanistic tasks in two differently prompted settings. By asking the instructors to *explain for themselves/think-aloud* we aimed at triggering an "expert frame" to elicit explanations, which they would give spontaneously to explain the mechanistic tasks for themselves without a teaching context. By changing the explicit instruction to a request to *explain to students*, we intended to trigger a "teaching frame" in which explanations are shaped to intentionally target fictitious students.

Research goals and questions

As the frameworks that characterize mechanistic reasoning were mainly used to analyze students' reasoning, little is known about instructors' approaches when explaining mechanistically. Instructors can be regarded as lynchpins to promote the

building of scientific explanations in students, and thus, we wanted to investigate how they shape their mechanistic explanations in order to generate implications for teaching Organic Chemistry. We wanted further insight into instructors' construction of cause–effect rationales. Specifically, we were interested in whether causes and effects are verbalized in relation to each other and whether different grain sizes are used in the rationales, *i.e.*, whether implicit information is used in addition to explicit features. Not much is known about how instructors verbalize logical sequences to make a claim when explaining mechanistic tasks and how they make use of the given representations in different frames. Further, we were interested in how instructors combine their cause–effect rationale with additional explanatory elements in an explanation, especially when targeting their explanations at students. This focus is intended to broaden the analysis of how cause–effect rationales are embedded by the instructors. Hence, we set out to analyze how different frames – an expert and a teaching frame – influenced instructors' explanatory approaches. The following research questions guided our investigation:

RQ 1: How do instructors make use of causes and effects when explaining case comparisons in an expert frame and in a teaching frame?

RQ 2: How does the use of causes and effects in instructors' mechanistic explanations change from an expert frame to a teaching frame?

RQ 3: How is the rationale combined with additional explanatory elements in the different frames?

Methods

Context and participants

The research was conducted at three German universities during the summer term of 2018. Ten instructors volunteered to participate in the study – nine male and one female (no other gender was mentioned). Seven of the ten instructors were leaders of Organic Chemistry research groups; the remaining three were affiliated to such research groups. All of the instructors were professors or lecturers teaching Organic Chemistry (beginner) courses following a traditional curriculum on a regular basis. Their teaching experience ranged from 11 to 30 years, with an average of 21 years. To protect the instructors' identity, they are given pseudonyms in this publication, randomly chosen from a list of the most common English surnames.

The research design followed ethical standards and all the participants were provided with information about their rights and the handling of the data (IRB approval is not a requirement at German universities). Participants were assured that they could opt out at any time during data collection. Furthermore, informed written consent was obtained prior to the data collection permitting the transcription of the interviews by the research team and/or a professional transcription service, data analysis conducted by the research team, and the use of the data for conferences and publications. The interviews were conducted in German and quotes were translated for this publication.

Instrument

To elicit instructors' reasoning, purposefully designed case comparisons were used as instruments (Graulich and Schween, 2018) (Fig. 1). These case comparison tasks have been shown to be a useful tool to elicit deeper reasoning and to weigh variables through comparison (Alfieri *et al.*, 2013). Such tasks have been used in the context of Organic Chemistry. For example, Watts *et al.* (2021) analyzed resources activated by students when reasoning mechanistically. Bodé *et al.* (2019) investigated students' ability to construct scientific arguments, and Caspari *et al.* (2018) analyzed the levels of complexity of relations that students constructed. Graulich and Bhattacharyya (2017) examined the categorization behavior of undergraduate students. Although these studies focused on students' mechanistic reasoning, we used case comparisons to elicit instructors' mechanistic explanations. The case comparisons used in this study address nucleophilic substitution reactions (Fig. 1), which are covered in beginner lectures of Organic Chemistry. The two cases, A and B, were purposefully contrasted in each of the tasks. They differed in one or two explicit differences, such as different leaving groups or backbones of substrates, which influenced the reaction rate. The instructors were asked to decide which reaction (of the two reactions shown) runs faster and to explain the reasons for their decision in two different frames, *i.e.*, to explain spontaneously for themselves and to explain for a fictitious student. This type of question, *i.e.*, to determine the faster reaction, is a typical mechanistic question proposed by Goodwin (2003) for Organic Chemistry. To draw a conclusion about which reaction is faster, one needs to consider which of the two reactions has a lower activation energy, which in turn is dependent on the potential energy of the transition states. Such conclusions about the transition states can be derived by inferring information from the structural formulas (Goodwin, 2003). Thereby one "[…] needs to form a bridge between structure and energy" (Goodwin, 2003, p. 144), *i.e.*, structural and energetic accounts must be connected (Goodwin, 2003; Goodwin, 2008; Caspari *et al.*, 2018).

For example, in task 1 the explicit difference of the structural formulas lies in the number of alkyl residues, *i.e.*, tertiary *versus* secondary alkyl substrate. When answering which reaction is faster, one would be asked to build a cause–effect rationale: when the leaving group departs, the higher number of alkyl substituents leads to more donation of electron density of σ_{C-H}-orbitals into the adjacent forming p_z-orbital and thus a better weakening of the partially formed positive charge in the transition state of A compared to B. Based on these structural considerations about the cause (hyperconjugation of alkyl residues) and effect (charge weakening) in the transition state, one can infer a claim about the activation energy or which reaction proceeds faster, *i.e.*, reaction A is being faster due to a lower potential energy of the transition state compared to B. Thus, an explanation to a case comparison can be expected to entail several causal relations, *i.e.*, structural causes and resulting effects on structural changes during the reaction within the

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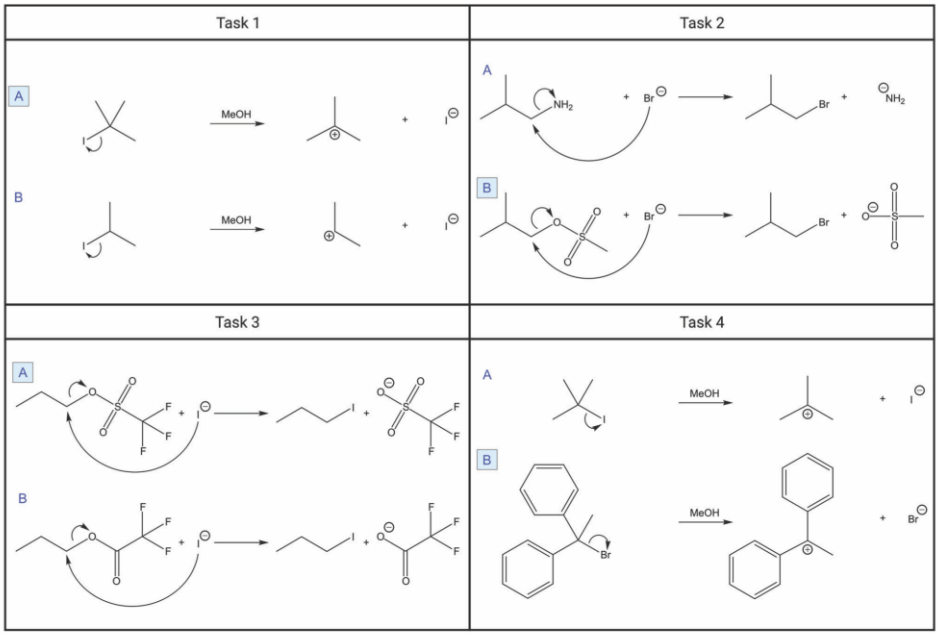

Fig. 1 Case comparisons used in the study. The reaction that occurs faster is marked in each task.

structural account. Furthermore, connecting links between the structural and energetic account can be expected to be established (Goodwin, 2003).

Tasks 1 and 4 both show the mechanistic step of a leaving group departure. In each case, a leaving group leaves an alkyl substrate in methanol under the formation of a carbocation and a negatively charged leaving group. Tasks 1 and 4 differ in the nature of the substrate, *i.e.*, tertiary (2-iodo-2-methylpropane) *vs.* secondary alkyl substrate (2-iodopropane) and tertiary alkyl substrate (2-iodo-2-methylpropane) *vs.* tertiary phenyl substrate (1-bromo-1,1-diphenylethane). Additionally, in task 4, the cases differ in the nature of the leaving group (iodide *vs.* bromide); therefore, this task has two explicit differences, *i.e.*, substrate backbones and leaving groups differ. Tasks 2 and 3 display a bimolecular nucleophilic substitution reaction (S_N2), in which a halide attacks the substrate and simultaneously the leaving group departs. In both tasks, the cases differ in the nature of the leaving group, *i.e.*, amide (azanide) *vs.* mesylate (methanesulfonate) and triflate (trifluoromethanesulfonate) *vs.* trifluoroacetate.

As linking structural causes and their effects in the structural account has been found to be challenging for students (Caspari *et al.*, 2018), in this study, we focus on instructors' structural account. Thereby we especially focus on how they make use of information inferred from the structural formulas and how they shape their explanations to make claims about energy.

Data collection

To collect the instructors' explanation within two frames, we conducted semi-structured interviews within a larger project on solving case comparisons in Organic Chemistry (parts published in Rodemer *et al.*, 2020). The instructors were interviewed individually and asked to solve case comparisons in two differently prompted scenarios. The case comparisons were displayed on a screen in the same order for each instructor. The instructors could decide for themselves when to move on to the next task. The interviews were recorded with an audio recording device.

In the first scenario, the instructors were asked to first mentally solve the task, by deciding which reaction occurs faster, and to explain their choice afterwards. We call this scenario the expert frame. Under this frame, the given prompt was: "In the following you will see the same reactions as before (while mentally solving the task). Describe the reactions and the differences between A and B. Let us know which reaction runs faster and explain the reasons for your decision." With this prompt, we wanted to trigger a spontaneous solving

behavior to elicit how the instructors would solve a task for themselves. This prompt was specified during the interview by asking the instructors to explain for themselves or a colleague, *i.e.*, to give an explanation for a knowledge level on an equal footing.

In the second scenario, the instructors were asked to explain the case comparison to a (fictitious) typical student who (hypothetically speaking) would participate in an Organic Chemistry I lecture of the instructor. We call this second scenario the teaching frame, in which we used the following prompt: "In the following you will see the same reactions as before (during spontaneously solving the task). Please explain which of the reactions runs faster to a student with low prior knowledge who takes part in your Organic Chemistry I course." The instructors went through all of the case comparisons at first in the expert frame, and were then given the second prompt of the teaching frame. Only instructors' direct responses to the tasks were included in the data analysis to capture their initial approach to explain the cases.

Data analysis

The interviews were transcribed verbatim and implemented into the coding software MAXQDA for qualitative content analysis (Saldaña, 2016). To further analyze the data, we followed four distinctive steps (Fig. 2).

Step I: identification of causes and effects

In the first step of analysis, the cause–effect rationales entailed in the structural account were analyzed. When explaining mechanistic problems, the rationale involves the part of the explanation in which reasons for the why are expressed. In each rationale, we were looking for verbalized structural causes and their effects within instructors' structural account. As each reaction step has an inherent cause and a resulting effect, one would expect that a rationale includes a cause, such as a property of an entity that leads to an effect in the process. A rationale, for example, could entail reasoning about the electron donating effect of the alkyl groups (cause) that weakens the positive charge of a resulting carbocation (effect). To identify which structural causes and resulting effects are used by instructors, we adapted aspects of the coding approach used for comparative mechanistic reasoning proposed by Caspari *et al.* (2018), as parts of their coding entailed the characterization of causes and effects. Caspari *et al.* (2018) differentiated between the use of explicit structural differences or implicit† structural properties used to verbalize a cause, and if either no effect, a non-electronic, or an electronic effect on a change in the process was described in a relation. Given our research focus on two differently framed situations, we used an adapted version of cause and effect categories to characterize instructors' use of causes and effects as the core of a structural account without coding complexity of relations.

† The term "implicit" refers to the inferences made from the representational level, *i.e.*, inferring meaning/conceptual knowledge

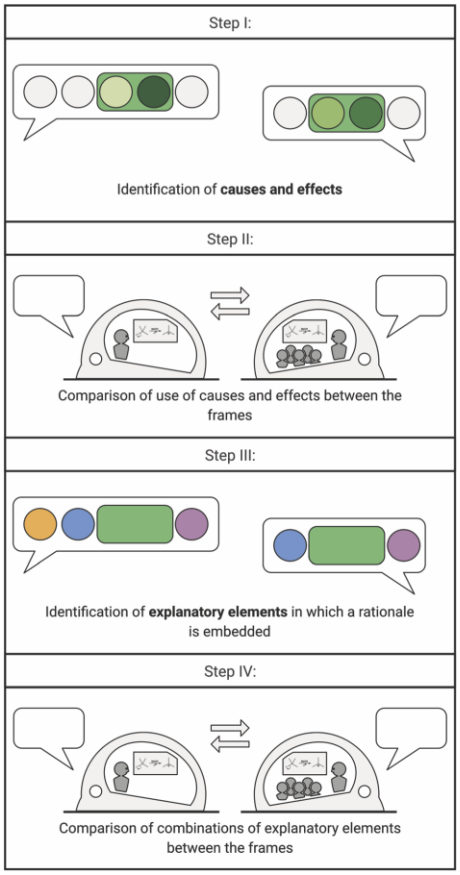

Fig. 2 Steps of the analysis. Green circles represent causes and effects. The green rectangle represents the rationale. Colored circles represent explanatory elements.

Besides identifying causes and effects, we also identified if causes and effects are combined (*i.e.*, complete cause–effect rationales) or if either causes or effects are mentioned separately (*i.e.*, incomplete cause–effect rationales). The counting of the rationales was done according to their content. For example, if an explanation for task 2 entailed reasoning about mesomeric effects and, in addition, about the acid strength to support a claim, two rationales were counted.

We used three coding categories to characterize the grain size of causes: *explicit*, *implicit*, and *implicit-electronic*. The assignment of these coding categories was determined by the use or non-use of implicit properties (Table 1). An *explicit cause* was given when an explicit structural difference, such as explicit surface features of the structural formulas, was used as a cause.

Table 1 Coding rubric for structural causes and effects on the reaction process

	Code	Code description	Example (referring to task 1)
Cause	Explicit	Participant refers to what is explicitly visible/to parts of the representation without inferring an implicit structural property	"...*because we have a tertiary carbon backbone as a substrate, instead of a secondary.*"
	Implicit	Participant uses an implicit structural property/names a concept	"...*because of hyperconjugation.*"
	Implicit-electronic	Participant refers to the implicit-electronic structure	"...*because with the tertiary carbocation ion there is more hyperconjugation due to more electron-pushing groups*"
Effect	Non-electronic	Participant verbalizes an effect of a structural cause without elaborating on the electronic level	"...*the product in A is more stable.*"
	Electronic	Participant verbalizes an effect of a structural cause with elaborating on the electronic level/charge distribution	"...*which leads to the positive charge being weakened.*"

The code *implicit cause* was given when an implicit structural property or concept (*i.e.*, which denominates a property) was used as a cause. The code *implicit-electronic cause* was applied when an implicit structural property was named and verbalized by referring to the electronic structure.

The analysis further focused on the structural *effects* on the course of the reaction. We used two coding categories to capture the differences in how a resulting effect was described: *non-electronic* or *electronic*. The assignment of the codes was determined by its reference to the electronic level, *i.e.*, when the effect of the implicit structural property was further explained using a reference to electron movement, overlap of orbitals, or charge distribution (Table 1). Instructors verbally expressed effects often as "being faster". However, these statements were not considered as effects in our coding, as they cannot be considered as structural effects directly related to a structural cause. We considered these statements as a part of a claim about energy that the task required. To us it was of interest how the structural account, *i.e.*, structural causes and their effects, was verbalized in an explanation to make a claim about energy.

Step II: comparison of use of causes and effects between frames

To compare the use of causes and effects between the frames, an exact test of symmetry (multinomial exact test) was performed. This test was chosen to determine the change or relatedness of frequency distributions of codes found in both frames, *e.g.*, to determine whether implicit causes in the expert frame were verbalized in the same way in the teaching frame or to determine whether there is a shift towards the other cause code categories. Therefore, the data were grouped by *participant*, *task*, and *content of the rationale (concept)* to identify if rationales (*i.e.*, causes and effects) appeared similarly, *i.e.*, referring to the same content in both frames. If a code was found within this grouping in one frame and no matching code was found in the other frame, it was coded with "none" in the other frame. Moreover, pairwise *post hoc* comparisons were performed to further draw conclusions about significance.

Step III: identification of explanatory elements in which a rationale is embedded

To characterize additional explanatory elements used by the instructors to accompany their rationales in mechanistic explanations, we derived three inductive categories. The additional explanatory elements included the *description of the process*, the verbalization of *general statements* and rules, and an outline of their problem-solving *approach* (Table 2). The code *description of the process* was chosen when the displayed reaction process was referred to, *e.g.*, if an instructor verbalized the formation of a charge or the bond breaking and formation.

The code *general statement* included the general description of properties (*e.g.*, of functional groups in general) and statements that are verbalized in a rule-based manner (*e.g.*, talking about the reactivity of entities in general). As instructors often explicitly stated how they approached a task, the code *approach* was derived. This code includes verbalization of strategies or problem-solving steps, such as hints to solve the task, *i.e.*, what to look for, what (and how) to compare, consider, weigh, or to distinguish something.

Table 2 Coding rubric for explanatory elements

	Code	Code description	Example (referring to task 1)
Explanatory elements	Description of the process	Participant refers to the displayed reaction process	"*We see two reactions here as competitive reactions in terms of speed. The reactions concern the leaving of identical iodide leaving groups from an alkyl; one is secondary and the other one tertiary...*"
	General statement	Participant verbalizes generalizations and rules	"*The reactivity for nucleophilic substitution reactions increases in general, in the case of S_N1, from primary, to secondary, to tertiary...*"
	Approach	Participant verbalizes an approach to solve the task	"*Now we have to look at the carbocations and weigh the stabilization of them against each other.*"

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Step IV: comparison of combinations of explanatory elements between the frames

In a fourth step, we analyzed how the explanatory elements were used in mechanistic explanations by the ten instructors while solving the four tasks in the expert and teaching frame. As we were interested in how instructors embed their rationales, we took a closer look at the sequential use of explanatory elements in their explanations, *i.e.*, how and if rationale, description of the process, general statement, and approach were used and combined in their explanations. Accordingly, we identified transitions made between the elements while explaining. Furthermore, we determined how often an explanatory element was used at the beginning of an explanation.

With the coding of causes and effects and the coding of additional explanatory elements, a complete categorization of the transcripts was achieved. During the qualitative analysis, the coding schemes (*i.e.*, causes and effects, explanatory elements) were constantly discussed between the authors to ensure that coding decisions faithfully represented the data. For inter-rater reliability, the first and the third author coded a random sample of 20% of the data independently. For the causes and effects coding rubric (Table 1), a Cohen's kappa coefficient of 0.88 was obtained and for the explanatory elements coding rubric (Table 2) a Cohen's kappa coefficient of 0.93 was calculated, indicating high agreement and reliability for both coding rubrics (Rädiker and Kuckartz, 2019).

Results and discussion

Here the mechanistic explanations of the instructors in two frames are compared and structured according to our three research questions. We focus on the comparison between an expert frame and a teaching frame to shed light on the potential flexibility of instructors when explaining mechanistic tasks. The use of framing illustrates that depending on the prompt, different expectations of an explanation can be triggered. In the following, we first focus on the characterization of structural causes and their effects. The second part reports how the use of causes and effects changed from one frame to the other. In the third part, explanatory elements used by the instructors are illustrated and it is shown how they were combined with the cause–effect rationales in both frames.

RQ 1: How do instructors make use of causes and effects when explaining case comparisons in an expert frame and in a teaching frame?

Causes and effects used in both frames

The distribution of causes and effects in instructors' structural account reveals differences between the frames; hence, differently shaped rationales were stated in both frames (Fig. 3). When prompted to solve the four case comparisons in the expert frame (Fig. 3, left), the ten instructors verbalized a total of 57 rationales. The causes used in these rationales differed with regard to the extent the instructors used implicit information, such as implicit properties. In the expert frame, we

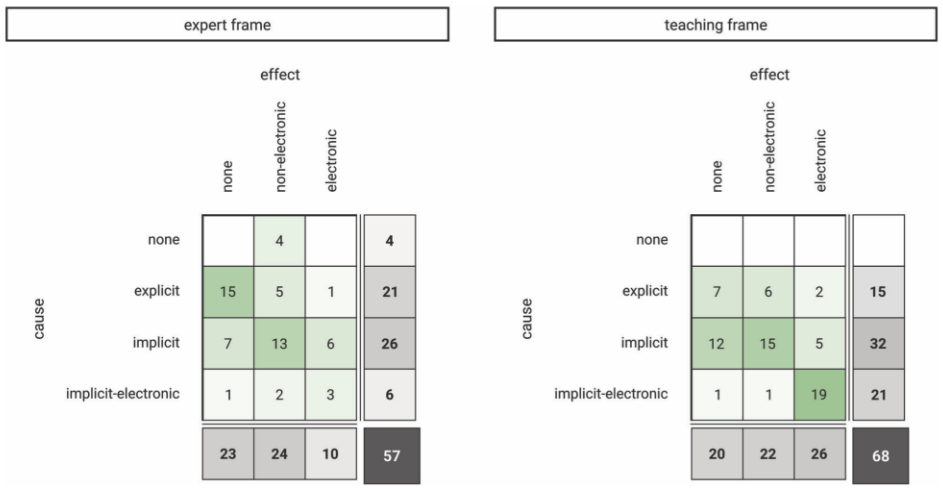

Fig. 3 Distribution and combination of cause and effect codes in the expert frame (left) and in the teaching frame (right); the darker the color, the more codes were identified. Green tiles represent the combination of cause codes (*y*-axis) and effect codes (*x*-axis), *e.g.*, in the expert frame (left) 5 explicit causes were stated in combination with non-electronic effects. Grey tiles represent the sum of each code category. Total number of rationales of ten instructors solving four tasks in each frame: expert frame = 57; teaching frame = 68.

identified 21 explicit causes, 26 implicit causes, and 6 implicit-electronic causes. Furthermore, 24 rationales entailed non-electronic effects and 10 rationales included electronic effects. As one would expect causes and effects to be verbalized relating to each other, we further analyzed if complete cause–effect rationales were formed. In 4 rationales, causes were missing as only an effect of a property was mentioned without referring to a cause of this effect, whereas in 23 rationales, an effect of a mentioned cause was not stated. Hence, nearly half of the rationales formed by the instructors in the expert frame were incomplete cause–effect rationales, stating either causes or effects and not both in relation, which corresponds to the prompt of the frame, which was to explain to themselves or a colleague. Beside instructors' use of structural causes and effects in the expert frame, we wanted to elicit how the instructors' cause–effect rationales are shaped when asked to target their explanation for a learner; if then, for instance, causes and effects are used more often in a fine-grained manner (*e.g.*, considering the electronic level) and if the construction of complete cause–effect rationales increases. When solving case comparisons in the teaching frame, the instructors used a total of 68 rationales to explain their reasoning (Fig. 3, right). The identified causes of the rationales were 15 explicit causes, 32 implicit causes, and 21 implicit-electronic causes. The identified effects of the rationales in the teaching frame were 22 non-electronic effects and 26 electronic effects. As in the expert frame, causes and effects were not always mentioned together in a rationale. In contrast to the expert frame, each rationale entailed a cause. However, in the teaching frame, nearly a third of the instructors' cause–effect rationales can be considered incomplete, as in 20 out of 68 rationales the effects of mentioned causes were missing.

It is noticeable that 57 rationales were mentioned in the expert frame while 68 rationales were mentioned in the teaching frame (Fig. 3). Prompting the instructors to explain to a fictitious student increased the verbalization of cause–effect rationales, as compared to the expert frame showing the possibility of adaption of the instructors to different addressees.

Cause and effect combinations in the expert frame

The most common combinations of causes and effects in rationales found in the expert frame (Fig. 3, left) show that instructors often relied on structural features, *i.e.*, explicit causes to back up their claim without mentioning an effect of a structural cause.

Instructor Franklin's rationale of task 4 illustrates this finding. In his explanation, he described the type of reaction and the backbones of the substrates in a bullet point manner without further elaborating on the effect of a structural cause, *e.g.*, a weakening of charge.

Instructor Franklin: *S_N1 substitution. Tertiary substrate versus twice benzylic tertiary substrate. B is faster by orders of magnitude.* (Task 4, expert frame)

Instructor Franklin compared the representational features (tertiary and secondary substrate), without referring to implicit properties, which corresponds to an explicit cause. Instructor Franklin verbalized "being faster" as a claim about energy which he linked to an explicit structural difference. He did not state further effects of structural causes, in terms of how the explicit differences of the backbones influence the reaction process. Thus, no effect of a structural cause was verbalized and coded within his explanation.

Verbalizing causes without effects, as found in instructor Franklin's statement, was identified in 40% of the rationales in the expert frame. This finding does not seem surprising if one considers the framing. In the expert frame, the explanations of the instructors appear to be short or abbreviated, which can be interpreted as instructors taking into account the knowledge of their addressees, *i.e.*, themselves or colleagues and thereby reflecting an expert's existing knowledge in Organic Chemistry mechanisms. Accordingly, instructors assume that addressees have the skills to infer implicit concepts and effects on the process from the comparison of structural features (*e.g.*, tertiary *vs.* secondary backbone). As literature suggest, experts are able to recognize important features, being able to make use of their structured cognitive resources, *i.e.*, their links to concepts (*e.g.*, Bedard and Chi, 1992). The instructors, thus, stated explicit structural differences as the linkage to certain concepts occurred naturally to them, respectively their addresses.

Other rationales (56%) went beyond the consideration of structural differences and included implicit information, such as naming of implicit structural properties or naming of concepts. These implicit causes were used most frequently in combination with non-electronic effects (Fig. 3 left), as illustrated by the explanation of instructor Evans for task 1.

Instructor Evans: *Yes, it's about splitting off from a leaving group and then a secondary and tertiary substrate form. In addition, the tertiary will almost certainly go better because it is better stabilized through inductive effects.* (Task 1, expert frame)

In his statement, instructor Evans acknowledged the explicit difference of the backbones (tertiary and secondary substrate) and further mentioned the inductive effects of the tertiary alkane as an implicit property (implicit cause). He also mentioned the resulting increase in stabilization, which was coded as a non-electronic effect. Instructor Evans's explanation could not be categorized as the most elaborated category of a cause, as a reference to the level of electrons was missing, *e.g.*, the positive inductive effects resulting from electron donation of the methyl groups, which would be categorized as an implicit-electronic cause. Implicit-electronic causes were used the least by the instructors in the expert frame.

Looking at use of effects in the expert frame, it was found that nearly half (24 out of 57) of the rationales entailed non-electronic effects, *e.g.*, see instructor Evans's rationale for task 1. In such rationales, effects were verbalized without a reference to the level of electrons, *i.e.*, often stating a stabilization without explaining how an implicit property electronically influences the course of a reaction. However, almost a fifth of the rationales entailed effects that were electronic in nature, *e.g.*, when instructors mentioned a weakening or distribution of a positive charge.

In the expert frame in general, the instructors' explanations were characterized by stating comparisons based on explicit structural features and naming of implicit structural properties to back up their claim without referring to the electronic level or inferring effects of structural causes. This shortened use of causes and effects in the expert frame resulted in nearly half of the rationales being incomplete, *i.e.*, in 23 out of the 57 rationales an effect of a cause was missing and in 4 out of the 57 rationales a cause of an effect was not mentioned. One could easily interpret these findings as a lack of sophistication, as a focus on explicit features mirrors the findings from studies based on student interviews. While students often focus on the surface of the representation and overlook implicit structural features (Weinrich and Talanquer, 2016; Graulich *et al.*, 2019; Moreira *et al.*, 2019a), the instructors' behavior of verbalizing explicit structural features and implicit information (while neglecting the electronic level) to back up a claim could rather be linked to their expert-like behavior. Literature suggests that Organic Chemistry experts, like the interviewed instructors, are able to engage in multivariate thinking due to internalized concepts and to conceptualize processes at a different representational levels (Bhattacharyya, 2008). Thus, the fact that the instructors often verbalized explicit features in the expert frame does not imply that they did not use their internalized concepts in their reasoning and do not have access to these resources. The verbalization of their reasoning was influenced by the prompt of the expert frame; accordingly, the framing may have led them to make use of their routinized expert response behavior that they use within their professional context and anticipate an expert's existing knowledge in Organic Chemistry. This behavior could be interpreted as not fully elaborating the "highest resolution" of reasoning, *e.g.*, by not mentioning cause–effect relations with a depth in grain size, or solely naming causes without effects. Talanquer (2013) commented on chemists' ability to make effective decisions, noting that they "rely on the thoughtful application of a variety of empirical generalizations used as heuristics or rules-of-thumb to make quick decisions" (Talanquer, 2013, p. 836). With this expert-like manner, they might have been able to go efficiently to the next task by quickly generating a claim.

The fact that the instructors did not verbalize their mechanistic consideration in detail in the expert frame, *i.e.*, on the grain size of electrons, could result from the instructors not considering this level of resolution to be appropriate or necessary in this context. Similarly, Weinrich and Talanquer (2016) concluded from their work on mechanistic reasoning: "that more advanced knowledge may lead individuals to build less sophisticated but more targeted and productive explanations" (Weinrich and Talanquer, 2016, p. 403). Since the framing of the prompt led the instructors to solve the task spontaneously, without further requirements for how elaborated the explanation should be, the instructors may have considered their explanations to be *productive* for this given context of explaining for themselves. Thus, verbalizing less detailed knowledge and using more short-cuts seemed reasonable to the instructors in this frame.

Cause and effect combinations in the teaching frame

As shown in Fig. 3 (right) for the teaching frame, the most frequent cause–effect rationale was the combination of implicit-electronic causes in combination with electronic effects. This finding can be illustrated by the excerpt of instructor Davis explaining task 4 in the teaching frame. In his rationale, instructor Davis recognized the explicit difference in the different backbones of the products (*tert*-butyl carbocation *vs.* diphenylethyl carbocation). He inferred implicit information and thereby considered electronic properties. He described how the p-orbitals can overlap and donate electron density to the empty p-orbital of the cation (implicit-electronic cause). He used this implicit-electronic property as a cause for an electronic effect by verbalizing how this leads to a delocalization of the positive charge and sharing of electron deficiency.

Instructor Davis: [. . .] *The second reaction is faster. This is due to the stability of the generated cation. The biphenyl substituted cation is more stable than the tertiary butyl cation, which we see in reaction A. And this is due to the two phenyl substituents. They contribute to the stability of this cation by donating electron density of the p-orbitals. The empty p-orbital of this cation [in B] can overlap with the p-orbitals of both phenyl rings and thus. . . positive charge is delocalized over 13 C-centers [carbon atoms]. Then each of them [the carbon atoms] has to carry only a 13th of the electron deficit load. Yes, this is what makes this cation so stable.* [. . .] (Task 4, teaching frame, excerpt)

In his rationale, instructor Davis not only named concepts and implicit properties, but described what this property means on a submicroscopic level, *e.g.*, the ability of phenyl substituents to donate electron density of the p-orbitals. Furthermore, concerning his verbalization of the effect of such a cause, he referred to delocalization and weakening of charge (electronic effect), which accounts for the stability of the diphenylethyl cation. As he elaborated on how the stability comes about by referring to the submicroscopic level, instructor Davis gave the term "stable" a greater depth of meaning. As his statement exemplifies, in rationales entailing the combination of implicit-electronic causes and electronic effects, concept designations and implicit properties were not only used as buzzwords, but were actually explained in an electronic and process-oriented way.

The second most frequent combination of causes and effects in instructors' rationales in the teaching frame was the use of implicit causes in combination with non-electronic effects. The excerpt of instructor Miller, as he explained task 1, exemplifies how implicit causes were used, often in terms of mentioning concepts, and in combination with non-electronic effects. As instructor Miller mentioned the inductive effect of the methyl groups, he referred to the implicit properties of an entity and thus the cause in his rationale was categorized as implicit. Furthermore, he mentioned how this structural cause leads to an increase in stability of the carbocation (non-electronic effect).

Instructor Miller: [. . .] *in one case it's a tertiary carbocation that forms, in the upper example, in the lower example it's a secondary carbocation. So, that's the difference. So the question of*

which of the two carbocations forms faster is related to stability. The more stable the carbocation, the faster it will form. And on the grounds of the +I effect of the methyl groups, which is stronger in the upper case than in the lower case, because we have three methyl groups at the top, which have a +I effect, and only two methyl groups with a +I effect at the bottom, therefore the upper carbocation is more stable and will also form faster. (Task 1, teaching frame)

Instructor Miller named the positive inductive effects in his rationale but did not further elaborate this concept at an electronic level, *i.e.*, describing the electron donation of the methyl groups. He then related this cause to an increased stability without mentioning what this means on the electronic level. This excerpt exemplifies a major finding, as nearly half of the rationales in the teaching frame entailed implicit causes, without referring to electronic properties and interactions on the electronic level.

The combination of implicit causes without an effect were found as often as the latter combination. This can be showcased by the quote of instructor Evans, while solving task 1 in the teaching frame. In his statement, he recognized the explicit difference of the different backbones of the substrates (secondary *vs.* tertiary), and referred to the inductive effect of the methyl groups (implicit cause), without further mentioning how these inductive effects influence the course of the reaction.

Instructor Evans: [...] *Due to the inductive effects by the three methyl groups, which have a stronger impact than in the lower case with the two methyl groups, we have a faster reaction progression in the case of a tertiary system.* [...] (Task 1, teaching frame)

Instructor Evans relied on naming inductive effects to back up his claim, without further explicating the effect, thus building an incomplete cause–effect rationale. Instructor Evans, among others, verbalized a qualitative statement of the inductive effects by stating that they have "a stronger impact". He did not further elaborate on this statement or provided an electronic effect to his structural cause, thus, missing to form a complete cause–effect relation.

Summarizing the instructors' explanations in the teaching frame, it is apparent that they often interpreted the prompt to explain to a student in a way that meant they elaborated more of what they might have not explicitly verbalized in the expert frame, which tributes to an increased number of rationales that could be identified in the teaching frame. Further, the instructors most frequently established causal relationships by verbalizing implicit-electronic causes with electronic effects. This increased depth in grain size in instructors' cause–effect rationales could be interpreted as an intention of instructors to provide a more detailed explanation and to support students to understand the mechanistic processes. As Ramsey (2008) states: "We have to be told where and why the electrons are moving in order for the mechanism to be explanatory." (Ramsey, 2008, p. 974). However, not all rationales stated in the teaching frame entailed an electronically justified cause–effect rationale, which would correspond to a high complexity of relation (Caspari *et al.*, 2018).

The findings show how instructors made use of causes and effect in the different frames. Further, the question arises where a change in elaboration of causes and effects has taken place.

RQ 2: How does the use of causes and effects in instructors' mechanistic explanations change from an expert frame to a teaching frame?

We further analyzed how the frequency distributions of the cause and effect codes from both frames relate, in terms of which codes relating to the same concept, and respectively content, can be identified in both frames and which codes differ. With regard to the 57 rationales verbalized in the expert frame and the 68 rationales verbalized in the teaching frame, only 37 rationales that were related to a particular concept appeared in both frames. Consequently, 51 rationales referring to particular concepts appeared in only one of the two frames (20 rationales in the expert frame and 31 rationales in the teaching frame). Rationales (*i.e.*, causes and effects) that were mentioned in only one frame were coded with "none" in the other frame, resulting in a total of 88 cause and effect codes in both frames. Based on these codes, we analyzed how each coded category appeared in both frames, *e.g.*, if all implicit codes of the expert frame occurred the same way (also as implicit codes relating to the same concept in the teaching frame) or if they were not mentioned, or shifted in their elaborateness in the teaching frame (Fig. 4).

Overall, the findings show a tendency towards an increase in grain size in both cause and effect codes, an increase in the use of causes and effects, and multiple rationales being verbalized in the teaching frame with different conceptual approaches.

In more detail, based on an exact test of symmetry (multinomial exact test), the cross table of cause codes (Fig. 4, left) can be considered non-symmetric ($p < 0.001$), indicating a significant change in the distribution of codes from the expert to the teaching frame with a large effect (Cohen's $g = 0.29$, (Cohen, 1988)). With regard to the absolute values, more implicit as well as implicit-electronic causes were mentioned in the teaching frame compared to the expert frame (Fig. 4, left). More precisely, it was found that 34 cause codes occurred equally in both frames (Fig. 4, left, sum of counters in diagonal tiles). In the teaching frame, 32 mentions of causes were found that were not mentioned in the expert frame (Fig. 4, left, bottom row; 3 counters at none/explicit, 16 counters at none/implicit, 13 counters at none/implicit-electronic), which refers to an increase in the use of causes in the teaching frame. Furthermore, as the cross table shows, 5 of the implicit causes used in the expert frame were verbalized as implicit-electronic causes in the teaching frame, hence, their elaborateness increased.

The cross table of effect codes (Fig. 4, right) is also non-symmetric ($p < 0.001$), again indicating a significant change in the distribution of codes from the expert to the teaching frame with a medium effect (Cohen's $g = 0.17$). Pairwise *post hoc* comparisons indicate that this change can be attributed predominantly to the increased use of electronic effects in the teaching frame ($p < 0.01$, Cohen's $g = 0.39$). In detail, 40 effect codes were verbalized likewise in both frames (Fig. 4, right, sum

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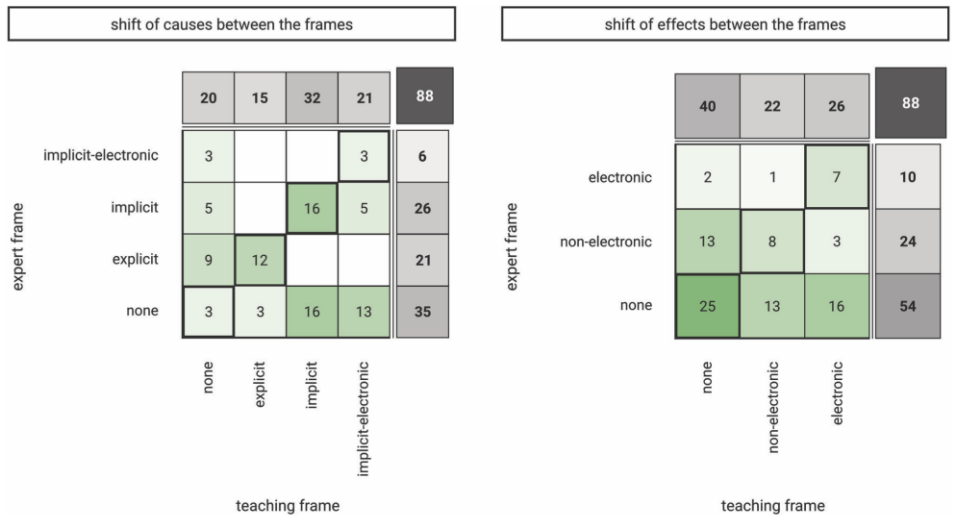

Fig. 4 Cross tables representing the distribution of cause codes (left) and effect codes (right) for both frames. The tiles of the cross table represent a match (thicker edged, diagonal tiles) or a shift of a code between the frames (*y*-axis: expert frame, *x*-axis: teaching frame).

of counters in diagonal tiles). In the teaching frame, 29 mentions of effects were found in the teaching frame that were not mentioned in the expert frame (Fig. 4, right, bottom row, 13 counters at none/non-electronic; 16 counters at none/electronic), which accounts for an increase in the use of effects in the teaching frame. Furthermore, while 1 electronic effect description in the expert frame occurred as a non-electronic effect in the teaching frame, 3 non-electronic effects occurred in the category of electronic effects in the teaching frame, hence, elaborateness increased.

The exact test of symmetry underlines the fact that there is a shift towards higher elaborated causes in the teaching frame (Fig. 4, left). Whereas, for the use of effects (Fig. 4, right), the number 25 in the lower left corner at none/none indicates that many rationales of the instructors entailed structural causes without a reference to effects of the reaction in the expert frame as well as in the teaching frame. Thus, the results for the effect codes indicate, however, a shift towards naming more effects in the teaching frame, especially electronic effects.

Robinson's explanation when solving task 2 in the expert and teaching frames clearly exemplifies a frame shift. Comparing his explanation in both frames shows differences in the usage and grain size of causes and effects. When solving task 2 in the expert frame, instructor Robinson states the explicit difference between the reactions, *i.e.*, the differing leaving groups: amide and mesylate. To back up his claim for reaction B being faster, instructor Robinson used a non-electronic effect, talking about the stabilization of the leaving group, without mentioning an implicit property as a cause for this stabilization or describing how the stabilization takes place.

Instructor Robinson: *So the lower one is faster because here we have two different leaving groups. One is an amine and then we have the amide that leaves. In the other one, it is the mesylate that leaves and in the mesylate, of course… well the leaving group is much better stabilized and the amide is just not [stabilized].* (Task 2, expert frame)

While solving task 2 in the teaching frame, instructor Robinson backed up his claim differently compared to the expert frame. In the first part of his explanation, he argued about what makes mesylate the more stabilized and therefore more favorable leaving group. He mentioned the mesomeric effect of mesylate, having electron pairs being able to "flip over" (implicit-electronic cause), and described how this results in the charge being distributed over the oxygen atoms (electronic effect).

Instructor Robinson: *Right. If we compare the reactions here, the difference is the leaving group. We simply have an amine at the top [reaction A] and mesylate at the bottom [reaction B]. This means that even if both reactions run by a S_N2 mechanism, we compare the different quality of the leaving group and thus we see how stabilized the leaving group is when it is split off. This means that we have the amide at the top [reaction A], accordingly, NH_2 minus, while we have the mesylate at the bottom [reaction B]. In the lower case, the negative charge can be distributed over all three oxygen atoms by simply flipping over the electron pairs. That means there is a strong mesomeric effect present and as you know, charged species are… the more you can distribute their charge… or the more atoms you can distribute it to, the more favorable.* […] (Task 2, teaching frame, part 1 of his explanation)

In contrast to the expert frame, instructor Robinson verbalized implicit-electronic properties for mesylate being the more favorable leaving group and described an effect of that structural cause including interactions on the electronic level. The frame shift, thus, resulted in a more elaborated cause–effect rationale for task 2. If we now look at the rest of his explanation when solving task 2 in the teaching frame, instructor Robinson added a conceptually different rationale to his first rationale by mentioning the acid/base properties of the leaving groups (implicit cause).

Instructor Robinson: [...] *This can also be directly correlated with the pK_a value. That means, the stronger the corresponding acid to the anion, the better the anion can be considered as leaving group. And if you now look at the pK_a value of the amine and compare it with the corresponding sulfonic acid... then you would immediately see that the amine is much less acidic, because amines react as a base after all and from this you can deduce that mesylate is the better leaving group and should be faster in B.* (Task 2, teaching frame, part 2 of his explanation)

In his further elaboration, instructor Robinson related the aforementioned cause–effect rationale and leaving group ability to the acid/base-strength. In this part of his explanation, he used implicit properties (pK_a values as a measure of acid strength, implicit cause). The differences in the completeness of the cause–effect rationales – as well as differences in the grain size of causes and effects – become apparent when comparing the frame shift. Frequent naming of implicit-electronic causes with electronic effects and implicit causes without resulting effects in the teaching frame were contrasted with the expert frame where explicit causes were often mentioned without an effect or with non-electronic effects.

Furthermore, instructor Robinson chose two different conceptual approaches in the teaching frame to underpin his claim. This increase in use of causes and effects in the teaching frame in contrast to the expert frame clearly shows that some instructors build multiple cause–effect rationales (*cf.* Table 3 in the Appendix) with additional conceptual approaches due to the frame shift.

In tasks in which more than one explicit structural feature differed (task 4) and the leaving group ability was discussed (tasks 2, 3, 4) instructors tended to use multiple rationales, *i.e.*, multiple conceptual approaches to underpin their claim. For example, like instructor Robinson's statement shows, the claim about energy was often asserted by two conceptual approaches: (1) a leaving group's capacity to distribute charge *via* resonance and (2) a statement about acidity. Noticeable is how the instructors were engaged in connecting their rationales. As instructors Robinson's explanation shows, he connects his two rationales by stating the mesomeric effect (cause) and the charge distribution in one anion (effect) "can also be directly correlated with the pK_a value" and relates to the corresponding acidity to the anion. By combining his rationales, he provided reasoning how acid/base-strength is related to mesomeric effects by referring to the capacity of charge distribution. He did not only provide two conceptual approaches but also showed how these are connected *via* the electronic structure, *e.g.*, capacity to accommodate charge, which is often found when instructors used multiple rationales.

Another example of an instructor's frame shift, which is comparable to instructor Robinson's explanation, can be characterized by looking at instructor Carter's explanations of task 3. In his explanation in the expert frame, he builds a cause–effect rationale stating that the difference in acidity (implicit cause) leads to a better stabilization of the trifluoromethanesulfonate ion (non-electronic effect).

Instructor Carter: *In both cases, the reactions are S_N2 reactions, without any doubts. The good nucleophile substitutes two leaving groups. However, the lower leaving group trifluoroacetate is still a bit worse than the upper leaving group, the trifluorosulfonate [trifluoromethanesulfonate]. This is because the trifluorosulfonate ion [trifluoromethanesulfonate] is even better stabilized than the trifluoroacetate ion and is therefore the weaker base. Conversely, trifluoroacetic acid is a stronger acid than trifluoromethanesulfonic acid, so the corresponding acid of the upper leaving group, is the stronger acid than trifluoroacetic acid.* (Task 3, expert frame)

In his explanation in the expert frame, he uses one conceptual approach (acid/base properties) (*cf.* Table 3). In the teaching frame, he adds another rationale by referring to resonance and the formation of contributing structures leading to a stabilization of the negatively charged leaving group. In this way, he provides more meaning to the used notion of "stability" relating it to the possibility of charge distribution.

Instructor Carter: *The upper reaction is faster because the forming negatively charged leaving group is better stabilized via resonance than in the lower case. In the upper case, you can formulate contributing structures [resonance structures]. In the lower case, there would only be two. And the possibility to formulate contributing structures which actually goes hand in hand, generally speaking, with stability of entities. One can check this by looking up the acidity of the corresponding acids. The corresponding acid in the upper case would be trifluoromethanesulfonic acid. And this is a stronger acid than trifluoroacetic acid. So, because of the fundamentally lower basicity and higher stability of the upper leaving group, the upper reaction is faster.* (Task 3, teaching frame)

By referring to resonance and acid properties, he, hence, uses two conceptual approaches in the teaching frame (*cf.* Table 3).

As a counterexample, we can consider instructor Davis, who only states one rationale in the teaching frame and names acid/base properties of the entities, which was coded as implicit cause.

Instructor Davis: [...] *The ability to be a good leaving group correlates with acid strength. Ammonia is a base, so we know, a very bad acid. Methanesulfonic acid, as the name implies, is a real acid, which means the stronger acid is methanesulfonic acid, so that is the better leaving group. Which meands reaction 2, B, is got to go much faster.* (Task 2, teaching frame)

In his statement instructor Davis relates the leaving group ability to the acid/base strength (implicit cause). Compared to instructor Robinson, he did not relate the leaving group ability to charge distribution, thus, he did not state an effect within his rationale and further only chose one conceptual approach, neglecting, *e.g.*, the mesomeric effects occurring in mesylate.

On the one hand, thus, one finds more elaborated cause–effect rationales in the teaching frame compared to the expert frame.

This result shows instructors' adaptability and underlines the fact that they are able to adjust their explanation depending on the framing. Considering causes and effects on a deeper grain size further highlights the instructors' tendency to step away from descriptive explanations, as implicit properties, the electronic structure of entities and its change in the course of the process are often included in their rationales in the teaching frame.

On the other hand, one finds an increase in use of causes and effects, which accounts for instructors often building multiple cause–effect rationales in the teaching frame. The latter appears to be a promising observation when thinking about providing students different conceptual approaches to a problem (*cf.* Table 3 in the Appendix). Results of a study looking at students' reasoning in mechanistic tasks by Bodé and colleagues (2019), show that incorrect claims were often stated when few connections among concepts were established (Bodé *et al.*, 2019). This suggests that strengthening links among concepts might be supported by instructors verbalizing multiple conceptual approaches.

However, in the teaching frame, even though instructors targeted their explanations for learners, in one third of their rationales causal relationships in terms of verbalizing structural causes *in combination* with their effects were neglected. Mentioning such causal relationships can be considered crucial for students in teaching contexts of mechanistic reasoning (Machamer *et al.*, 2000; Cooper, 2015; Crandell *et al.*, 2018). At the same time, the instructors may have implicitly considered more than they explicitly expressed when building their explanation and verbalizing the grain size of causes and effects. Bodé and colleagues (2019) stated in this regard that "an expert may have the *ability* to continue expanding their explanation or argument to ever decreasing levels of granularity, the *actual* granularity of their scientific explanation or argument, even a multicomponent, causal one, will depend on their context and purpose" (Bodé *et al.*, 2019, p. 1072). This may also account for the findings in our study.

This aspect of flexibly adjusting an explanation was as well brought up by instructor Smith in a side comment, after the expert frame:

Instructor Smith: *If you ask about the speed of the reaction, then you would have to work with the activation energies and I cannot just say 'the more stable cation is formed, therefore it reacts faster'. It depends on which level of explanation I adapt. So, in school, that is certainly how you would explain it. Um. In an introductory organic chemistry course, I would work with energy diagrams to correlate the transition state with the product, in this case [referring to task 1] the cation, according to the Hammond postulate for this exothermic step.*

He expressed his awareness that his brief statement given in the expert frame needs to be adapted to the respective level of knowledge of the learner by stating more implicit information, *e.g.*, on the reaction process. He then discussed the energetic process of the reaction in relation to structural properties, when providing his explanations in the teaching frame. Beside the trend of making more implicit information explicit due to the frame shift in our study, there is still great variety in instructors' use of cause–effect rationales in these two frames over all tasks. The latter points to the necessity of supporting instructors to become aware of how they are forming explanations and when to purposefully change the explanation in different contexts. Whereas some instructors decided to use more implicit information with regard to the frame shift, others did not change the way they verbalized their cause–effect rationales between the frames. Instructor Jones, for example, does not elaborate on the cause he uses in the expert frame explaining task 3 in the teaching frame. In both frames, he refers to the quality of the leaving groups to make a claim, which was coded as an explicit cause.

Instructor Jones: *Here the leaving group differs. Once a trifluoroacetate in case B. And in case A a trifluoromethanesulfonate. Both are S_N2 reactions. The trifluoromethanesulfonate is the better leaving group than the trifluoroacetate. And therefore, A will proceed faster than B.* (Task 3, expert frame)

In the teaching frame, he uses the same cause as in the expert frame.

Instructor Jones: *Here we have a case of a primary substrate with two different leaving groups, the nucleophile is the same, the leaving group is once a sulfonate and once a carboxylate, the residues with the CF_3-group are also still the same, which means we have to distinguish between sulfonate and carboxylate. Sulfonate is the clearly more stable anion and the better leaving group and that means that case A is faster than case B.* (Task 3, teaching frame)

Compared to the expert frame, he added a non-electronic effect as he claims the trifluoromethanesulfonate is being more stable. Even though he does not use more implicit properties as a cause in the teaching frame compared to the expert frame, he forms a complete cause–effect rationale, describes how one should approach the task ("we have to distinguish") and adapts his language to the frame. In comparison to the expert frame, he no longer uses a sophisticated nomenclature of the leaving groups, but the name of the functional groups, thus, building a bridge towards generalization or possibly simplification for a fictitious student. As the example of instructor Jones illustrates, it is not only worth looking at causes and effects, but also further aspects of the given explanation that might change through a frame shift, which are possibly influencing learning.

RQ 3: How is the rationale combined with additional explanatory elements in the different frames?

Explanatory elements identified in both frames

After discussing instructors' use of causes and effects, we analyzed how cause–effect rationales are embedded in the explanatory context when the framing changes. The inductive content analysis of instructors' explanations revealed three additional categories of explanatory elements, besides the rationale, *i.e.*, *description of the process*, *general statement*, and *approach* (Fig. 5).

In the expert frame 57 rationales were verbalized by the instructors and in the teaching frame 68 rationales were mentioned. The identified explanatory element of *description of the process* was categorized 34 times in the expert frame and 60

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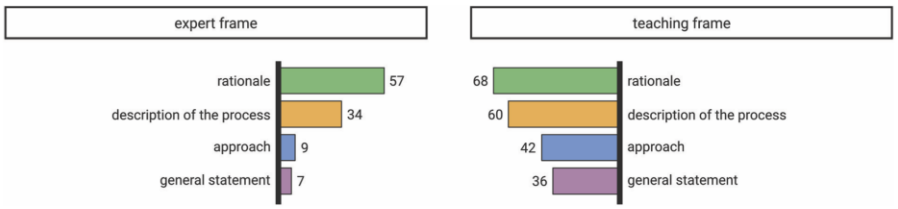

Fig. 5 Identified explanatory elements in instructors' explanations for 40 tasks in the expert frame (left) and for 40 tasks in the teaching frame (right).

times in the teaching frame. Furthermore, the category of *approach* was found 9 times in the expert frame and 42 times in the teaching frame. *General statements* were categorized 7 times in the expert frame, whereas they were mentioned 36 times in the teaching frame.

Comparing the use of explanatory elements, an increase from the expert frame to the teaching frame is apparent. This does not seem surprising if one assumes that the instructors adapted their initial explanation due to shifting towards a teaching context. When explaining in the teaching frame they tended to include additional elements in their explanation, influenced by what they thought might be beneficial in a learning context.

Embedding of rationales with explanatory elements in both frames

To further analyze how instructors embed their rationales, we took a closer look at the combination with the explanatory elements and analyzed their sequential use (Fig. 6).

In the expert frame, the rationale was often accompanied by a *description of the process* (Fig. 6, left, width of yellow and green chords transitioning between *description of the process* and *rationale*). Thus, the beginning of an explanation often started with the *description of the process* (Fig. 6, left, height of the yellow node) followed by the verbalization of the *rationale*. This common occurrence is illustrated with instructor Lewis's explanation, as he explained task 1 in the expert frame. He started his explanation with a short description of the mechanistic step of leaving group departure, *i.e.*, which was categorized as *description of the process*.

Instructor Lewis: *We have two reactions, in which an iodide leaves an alkane, forming a positively charged carbon atom.* [...] (Task 1, expert frame, description of the process)

After the description of the leaving group departure, he verbalized his rationale, in which he stated an explicit cause (*i.e.*, tertiary *vs.* secondary carbocation) and a non-electronic effect (*i.e.*, better stability).

Instructor Lewis: [...] *The difference is that it is a secondary and a tertiary [carbocation]. In the upper case, the positive charge is significantly better stabilized than in the lower one, the rest is the same. The upper one should be formed faster because of the better stability.* (Task 1, expert frame, rationale)

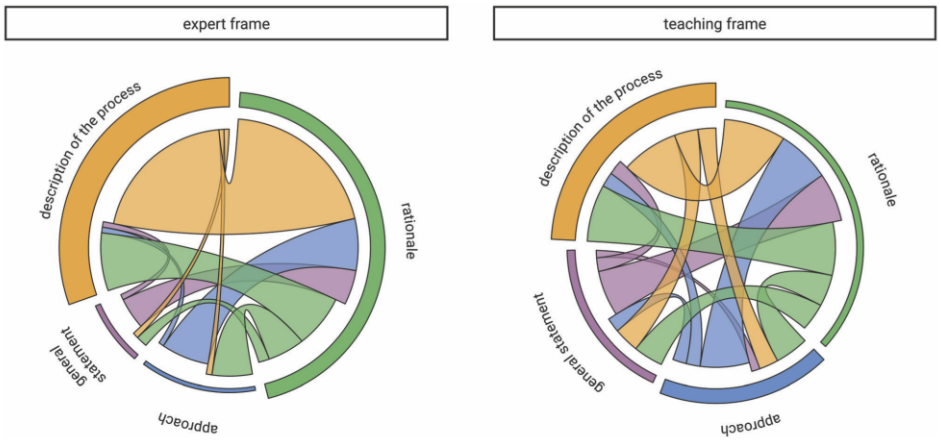

Fig. 6 Relative numbers of transitions between explanatory elements in the expert frame (left) and in the teaching frame (right). The proportions of the outermost ring indicate the relative frequency of the reference to an explanatory element. The height of the outermost ring (node) indicates how often an explanation was started with the respective explanatory element. The width of each chord represents the frequency of transitions made between respective explanatory elements; indented chords symbolize a transition from one explanatory element to another.

Compared to the frequent combination of *description of the process* together with the rationales in the expert frame, the categories *approach* and *general statement* were combined less frequently with the rationales (Fig. 6, left, widths of the blue and purple chords between the respective explanatory elements and the *rationale*). As the expert frame was meant to explain to colleagues or themselves, it is not surprising that the instructors tend to connect their rationale only with few explanatory elements. These findings again indicate a pragmatic approach in the expert frame, as the instructors focused on the description of what was going on and stating their reason, when spontaneously solving a case comparison, rather than mentioning their problem-solving approach or general rules and statements.

Similar to the expert frame, the rationale in the teaching frame was often accompanied by a *description of the process* (Fig. 6, right, width of the yellow and green chords between the *description of the process* and *rationale*). Further, the *description of the process* was also often the beginning of an explanation (Fig. 6, right, height of the yellow node). When explaining to a fictitious student, rationales were typically accompanied by *general statements* and problem-solving *approaches* (Fig. 6, right, blue and purple chords between the respective explanatory elements).

Instructor Lewis's explanation of task 1 in the teaching frame illustrates this usage and frequent sequence of explanatory elements in explanations. In his explanation, he started with a *description of the process* as he referred to the departure of the leaving group and the formation of a carbocation.

Instructor Lewis: *It is about the separation of the identical iodide leaving group from an alkyl, one is secondary, one is tertiary. An energetically much higher carbocation is formed. This means that the carbocation is then an intermediate stage, an intermediate product.* [. . .] (Task 1, teaching frame, description of the process)

After describing the leaving group departure, he stated an *approach*, by describing what one needs to consider first.

Instructor Lewis: [. . .] *And now let us first consider the energy of these two intermediates*: [. . .] (Task 1, teaching frame, approach)

After he expressed where the focus must be placed first to solve this task, he went on to add a *general statement* about how stabilization of compounds is achieved in general *via* electron donation.

Instructor Lewis: [. . .] *It is an electron-deficient compound. In general, stabilization is achieved by residues that can supply electrons in some way; be it through mesomeric effects or inductive effects.* [. . .] (Task 1, teaching frame, general statement)

He stated his *rationale* by considering inductive effects of the methyl groups (implicit cause) being able to stabilize the positive charge (non-electronic effect).

Instructor Lewis: [. . .] *We do not have mesomeric effects, we only have inductive effects through the methyl groups. Above we have three methyl groups, which could stabilize this electron deficiency compound, this positive charge, below we have only two.* [. . .] (Task 1, teaching frame, rationale)

Instructor Lewis's explanation exemplifies a common sequence of explanatory elements in the teaching frame, in which first the reaction process was introduced, then an *approach* to solve the task was stated and a *general statement* was inferred before giving the *rationale*. As chords (and their widths) between the explanatory elements as well as the height of the outermost ring (node) in Fig. 6 (right) indicate, additional sequences and combinations of explanatory elements could be identified and, thus, the rationales were embedded differently.

Beside the *description of the process*, the problem-solving *approach* was frequently used at the beginning of an explanation (Fig. 6, right, height of the blue node). Instructor Miller, for instance, used an *approach* at the beginning of his explanation for task 2 in the teaching frame.

Instructor Miller: *Well, to determine which reaction is faster, we have to rely on the quality of the leaving group.* [. . .] (Task 2, teaching frame, approach)

In his statement, instructor Miller started with an *approach* of how one can tackle the question to answer which of the two reactions proceeds faster. Then, he made a *general statement* by correlating the stability of a leaving group with the stabilization of the negative charge.

Instructor Miller: [. . .] *And it is like this: the more stable a leaving group, the better the negative charge can be stabilized.* [. . .] (Task 2, teaching frame, general statement)

He then went on by stating an *approach* of how one can find out which of the leaving group is the better stabilized one, *i.e.*, looking at the structure.

Instructor Miller: [. . .] *And you can tell this either by looking at the structure and recognizing that* [. . .] (Task 2, teaching frame, approach)

Afterwards, he stated his *rationale* by acknowledging the (de)localization of charge. Compared to instructor Lewis in the teaching frame, instructor Miller did not start his statement with a *description of the process* but with an *approach* to the problem. He guided a fictitious student through the task by explicitly explaining a strategy to solve the tasks, using forms of direct address several times (''we''/''you'').

As shown by the explanations of instructors Lewis and Miller in the teaching frame, instructors used *general statements* and explained their *approach* frequently. Through general statements and rules, instructors might have intended to structure their explanation by first verbalizing something general and afterwards giving a specific example of how the general statement referred to the given task, *e.g.*, *''The reactivity for S_N1 reactions increases from primary to secondary to tertiary alkyl groups. In this case we have a tertiary butyl cation versus. . .''*. However, it is known that students tend to overgeneralize general statements and rules, *e.g.*, overgeneralizing definitions of reactions when classifying reactions (Stains and Talanquer, 2008) or when applying the octet rule (*e.g.*, Taber, 1998; Luxford and Bretz, 2014). The overemphasis of general statements in teaching situations may promote the reliance of rule-based reasoning, focusing on a single variable, in cases in which multiple variable thinking would be necessary (Kraft *et al.*, 2010; Talanquer, 2014). By stating *approaches*, the instructors might have intended to guide learners or to

highlight their approach by explicitly verbalizing ways to come to a problem solution. However, it should be noted that the identified *approaches* of the instructors differ. While some of the verbalized approaches might be potentially helpful for learners by stating the concepts or train of thoughts necessary to make a claim, others may not, as they trigger a pattern recognition based on representational features ("looking at the structure and recognizing that…") and might therefore promote heuristic reasoning. Both frames also revealed the frequent use of the *description of the process*. In teaching contexts, this could be beneficial for learning, as it goes beyond a static description of entities (*e.g.*, a product-oriented approach) and could support reasoning about the dynamic processes of mechanisms.

The characterization of explanatory elements provided further information on how the instructors constructed their explanation in the expert and teaching frames, and how they embedded the cause–effect rationale. While the *rationale* in the expert frame was frequently accompanied by a *description of the process*, in the teaching frame *general statements* and *approaches* accompanied the *rationale* more often and more transitions were made between the explanatory elements. The expert frame was found to trigger short-cut response behavior, while the teaching frame led to stating additional explanatory elements that instructors might believe to be necessary in a teaching situation. When explaining to fictitious students, the instructors integrated more *approaches* and *general statements* in their explanations. Although more explanatory elements were found in the teaching frame compared to the expert frame, this does not mean that the verbalization of an explanatory element would necessarily result in a benefit for learning. While some generalizations made through *general statements* could lead to a better structuring of an explanation, they could also promote an overgeneralization. Hence, general statements that regard implicit causes and effects (*e.g.*, relating stability to charge distribution like instructor Lewis did solving task 1 in the teaching frame) might be more beneficial in a teaching context than general statements regarding the explicit level (*e.g.*, designating the reactivity order based on the backbones of the substrates).

It remains to be seen whether certain explanatory elements, combinations, or transitions between them support students' learning in a more meaningful way than others do. At this point, the mere and multiple naming of explanatory elements should not be regarded as helpful *per se*, as qualitative differences within the codes could be identified (*e.g.*, in how approaches are verbalized).

The differences found in the use of the explanatory elements in both frames, thus, may not seem surprising, as *framing* is considered to be an individual process and each instructor gave individual explanations of what they felt was appropriate in the given fictitious context (Berland and Hammer, 2012). To be more certain how to meet the prompt, the instructors often asked about the requirements of the situation of the respective frames. For example, instructor Miller asked for a feedback on his brief explanation after stating his answer to task 1 in the expert frame:

Instructor Miller: *That was a very brief explanation. Is that enough for you? So, I mean, that would now be my explanation for a colleague, so to speak. I mean to a student I would explain: You see the same leaving group. It is a S_N1 reaction… [goes on more in depth with his explanation]. So that would now be the explanation for a student, so to speak, in an organic chemistry beginner course.*

Interviewer: *Exactly, that [explaining to a fictitious student] will take place in the next scenario.*

By explicitly ascertain the requirements, the instructors were able to frame the situation respectively, which allowed us to draw conclusions about their shift in the explanations.

In addition, the framing was specifically ascertained by the interviewers, *e.g.*, by asking whether this explanation was shaped for themselves or a colleague, respectively a student with low prior knowledge.

At the beginning of the teaching frame, instructors further mentioned to aim at giving an explanation in a didactic way. After giving the prompt of the teaching frame, instructor Lewis, for example, ensured himself if there is time for doing so.

Interviewer: *Now we go on with your explanation [in the teaching frame].*

Instructor Lewis: *Okay. But I still have time to prepare for it, to explain in a didactically meaningful way?*

Interviewer: *Of course. But the task format is the same like before [in the expert frame].*

Instructor Lewis: *Okay, sure. Still, I think there [in the expert frame] I was thinking more for myself, so to speak, and not thinking about how to get there in a meaningful way.*

His statement further indicates that his framing has shifted from "thinking for himself" to aiming at thinking and explaining in a structured, meaningful way in the teaching frame, which was intended by the prompts. As illustrated before, instructor Lewis intentionally, thus, shaped his explanation to show how to come about to make a claim – "how to get there", *e.g.*, by considering the process and verbalizing approaches.

Limitations

A limiting factor of this study is that task effects were not considered in the analysis, *i.e.*, if small changes in the task design, such as differing substrates or differing leaving groups, change the shape of the explanation. This analysis would have been based on a very small sample size and thus we decided to consider the four tasks together. Another limitation is the number of instructors interviewed. This was limited due to the rank sought for the study, *i.e.*, Organic Chemistry research group leader and/or lecturer for Organic Chemistry beginner courses. Another limiting factor may result from the fictitious situation (*e.g.*, explain to a fictitious student) in which we placed the instructors. Direct addresses to students in the teaching frame (see instructor Miller, task 2, teaching frame) show that the instructors often adapted their explanation specifically to students, *i.e.*, they intentionally shaped their explanation in this way. Our data, however, were not collected in an authentic situation. The study therefore does not cover the social

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aspects or the spontaneity of a teaching situation. Investigations of how instructors react in authentic teaching settings would be useful to gain further insights into their construction of explanations. Furthermore, our prompt was to direct instructors' explanation to a fictitious student with low prior knowledge. We did not collect any data about students' prior knowledge in the classes of the instructors. Not regarding specific students' prior knowledge in our prompt was meant to create a consistent set of conditions for all of the instructors. Our focus of analysis therefore drew attention to each instructors' interpretation to the same prompt. Analyzing instructors' explanations targeted for different prior knowledge of students remains part of further investigations. In this regard, specific emphasis could be placed on how students respond to the use of multiple conceptual approaches and whether these prove to be beneficial to learning. Furthermore, to analyze an individual instructor's framing in detail one could investigate how an instructor would embed an explanation in the teaching context, *e.g.*, what would have been conceptually covered prior to instruction by the instructor.

The instructors were prompted in a way to frame a situation – first to explain spontaneously and then to explain to a fictitious student with low prior knowledge. These prompts were used for all four tasks. This may have influenced the generation of explanations going from one task to the other, as the instructors first had to complete the tasks in the expert frame and then again in the teaching frame. Although we have not observed a pattern that indicates such a sequence effect, it may have influenced instructors' decisions. Further, the task format of comparing two reactions in case comparisons, compared to common predict-the-product task, might have influenced instructors' approaches. However, the instructors self-reported at the end of the interview to use case comparisons in their classes, when teaching reactivity orders of single entities and did not report to have had struggled with the task format.

Additionally, to answer our research questions, we focused on the most common trends of instructors' mechanistic explanations triggered by a frame shift. Therefore, how individual instructors performed and whether individual explanations remained stable across frames were not described. However, this layer might provide further insights on instructors' approaches.

It can further be assumed that most instructors were unfamiliar with the demands and structure of mechanistic reasoning described in chemistry education literature. The categories of causes and effects defined in our study were not directly communicated to the instructors. Accordingly, they verbalized their explanations in a way which they thought might be adequate – which was what we intended by promoting a certain frame. For example, the pure verbalization of a stability difference was consistently categorized as a non-electronic effect. The instructors, of course, could have implied either reasoning about an electronic stabilization (structural account) or stability in terms of a thermodynamic attribution (energetic account). Further prompting could have revealed the core of the possibly implied variety of meanings of some terms, but would have additionally biased the intended framing and might have influenced the subsequent tasks.

Conclusions and implications

In this study, instructors' explanations of case comparison tasks in two differently prompted scenarios were the focus. We designed our instrument to tap into instructors' abilities to adapt their explanation to a specific context or frame (Tannen, 1993; Hammer *et al.*, 2005) – an expert frame and a teaching frame.

Our findings revealed that the expert frame led the instructors to favor a short-cut explanatory approach, which was shown, *e.g.*, in verbalizing causes without an effect. Further, they often did not involve the electronic structure and electronic interactions in their cause–effect rationales. These findings correspond to instructors taking the knowledge of their addressees into account, *i.e.*, anticipating an expert's existing knowledge in Organic Chemistry mechanisms and abilities to infer implicit information. In the teaching frame, the rationales of the instructors were frequently more elaborated compared to the expert frame, as more implicit information was verbalized and often multiple and complete cause–effect rationales were established, which is a promising finding and showcases instructors' adaptivity. Not all of the explanations given in the teaching frame, however, entailed an electronically justified cause–effect rationale, which would correspond to a high complexity of a relation. As Caspari and colleagues (2018) stated concerning the complexity of relations, "A more complex relation [with an electronically justified cause and effect] is not necessarily any better (or worse) than a less complex one. The advantage of a less complex relation is that it can be more easily communicated than a complex relation and enables faster decision making" (Caspari *et al.*, 2018, p. 1130). Thus, by stating less complex cause–effect rationales, the instructors could have attempted to facilitate understanding by communicating their reasoning in a less complex way. If one takes another look at the verbalized causes in the expert frame as well as when the instructors specifically targeted the explanation for a fictitious student, it was found that causes were often verbalized as a pure naming of implicit properties, *i.e.*, rather as verbalisms and buzzwords (*e.g.*, "is a weak base, therefore [. . .]"). In teaching contexts, students might adapt these vague verbalizations, which might hinder their meaningful learning and should be treated with caution. It has been shown that students tend to rely on verbalisms and therefore tend to engage in rote learning without having a deep understanding of the verbalism (Bhattacharyya, 2008). Furthermore, breaking down explanations to, *e.g.*, "good or bad" leaving groups or "strong or weak" acids in a teaching situation may cause learners to remain in dualistic thinking rather than considering multiple variables and reaction conditions (Popova and Bretz, 2018). As Popova and Bretz (2018) showed in their study of Organic Chemistry students' perceptions of leaving groups, less than half of the students were able to refer to the electronic and structural features that characterize a leaving group as "good". In their explanation, students found it difficult to name the implicit properties and to use them in a meaningful way to draw a conclusion. They typically relied on reciting examples of good and bad leaving groups that were presented during their lecture

(Popova and Bretz, 2018). This suggests that the mere naming of implicit properties or concepts as buzzwords in a teaching context may encourage the use of heuristics in students as well, in terms of verbalisms that cover up the lack of deep understanding of chemical concepts.

We found that in the teaching frame instructors often verbalized multiple rationales with different conceptual approaches. In a teaching context, it would be valuable to explain how different concepts can be related. What was found in our data was promising as instructors often connected different conceptual approaches of rationales, *e.g.*, resonance and acidity/basicity, in drawing back references to the (change of the) electronic structure, *e.g.*, the capacity to accommodate charge.

Further, our results showed that in both frames the instructors often verbalized their final answer to the case comparisons as a pure qualitative statement, *i.e.*, "has a stronger impact", "is better", "is weaker". In doing so, instructors did not address the effect of a structural cause of the reaction on a structural level and remain vague about the source of this qualitative difference. In teaching context, a pure statement of qualitative differences could result in students memorizing these differences without deeper understanding. Purposefully verbalizing the effect on the structural change allows to fill this missing link between the structural cause and the claim about energy or qualitative differences. Hence, if instructors attempt to explain a change in energy in a mechanistic task, the structural cause with its effect on the structural change needs to be considered in order to make a causally founded claim (Goodwin, 2003; Caspari *et al.*, 2018). To explain a case comparison that asks for a comparison in reaction rates, structural account and energetic account have to be connected by referring to both, cause and effect, in the structural account. While we have shown that instructors are able to shift between levels of details and grain size in an explanation, in the case of students, it may not be the same question of deciding which grain size of an explanation to use or being aware of it. Rather, it may reflect their actual understanding. Building well-grounded cause–effect relations needs support, for instance through explicit prompting or scaffolding. Students can be engaged in considering the electronic structure and building more elaborate relations, even in situations in which transfer of knowledge is needed (Caspari and Graulich, 2019; Crandell *et al.*, 2020). This emphasizes the importance of instructors' roles in purposefully supporting students to consider causes and effects with a reasonable grain size when teaching and verbalizing mechanistic reasoning.

The further analysis of instructors' mechanistic explanations revealed the use of explanatory elements, *i.e.*, *description of the process*, *general statements*, and *approaches*. These elements were used differently to embed the rationales in both frames. For example, while some of the verbalized *approaches* state the concepts or train of thoughts beneficial for problem-solving, others could trigger pattern recognition when only superficial features of a reaction are noted to be taken into consideration. A supportive approach could therefore rather be verbalized by stating how and where to derive implicit properties from the explicit features of a mechanism. Thereby, the formation of cause–effect rationales could be supported in terms of explicitly verbalizing the necessity to use implicit properties as structural cause for an effect to be able to make claims about energy. Hence, it remains to be investigated whether a certain embedding of rationales and use of explanatory elements (of a certain quality) is beneficial to promote students' mechanistic reasoning. Further research could be conducted taking the learning gains of students into account when they are "confronted" with a certain explanation.

Based on the analysis of instructors' mechanistic explanations, it was possible to pose implications, which consider students' challenges in building well-grounded explanations reported in the literature, *e.g.*, students' challenges in building cause–effect relations (Weinrich and Talanquer, 2016; Caspari *et al.*, 2018; Moreira *et al.*, 2019a) or in inferring implicit information (Bhattacharyya and Bodner, 2005; Strickland *et al.*, 2010; Anzovino and Bretz, 2016). Overall, we are aware that instructors' explanations are not solely responsible for learning and explanations constructed by students. An instructor's elaborate, causal explanation presented to students does not mean that this explanation is transferred to students' minds and that in turn the students are able to construct causal explanations themselves. Nevertheless, as students' challenges when reasoning mechanistically are well researched and the impact of an instructor's expressed mechanistic reasoning on students' mechanistic reasoning has already been shown (Moreira *et al.*, 2019b), instructors should be aware of their important role in the learning process. Based on our findings, the following aspects should be considered when instructors engage in mechanistic reasoning in teaching contexts: (1) formation of complete rationales in which structural causes and associated effects are verbalized; (2) when using multiple rationales, *i.e.*, multiple conceptual approaches, interrelating links should be made in terms of considering (the change of) the electronic structure; (3) when stating *general statements* focusing less on generalizations based on explicit differences, rather generalizable implicit-electronic relations should be stated; (4) making problem-solving *approaches* explicit. These aspects have the potential to be supportive when teaching Organic Chemistry, yet they must always be adapted to the specific student cohort's needs and prior knowledge. Hence, instructors should be aware of the complexity of the cause–effect relation, *i.e.*, the grain size of causes and effects, they verbalize and of what the untargeted verbalization of additional explanatory elements might trigger in learners (*e.g.*, structuring *vs.* overgeneralization; teaching problem-solving strategies *vs.* promoting pattern recognition). Our study revealed that instructors are engaged in customizing their explanation according to the frame, which illustrates their flexibility in adjusting or elaborating their mechanistic explanation. Whereas in the past, students' challenges were often the focus in studies, our study showed it is worth considering instructors' explanatory approaches.

Conflicts of interest

There are no conflicts to declare.

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Appendix

Table 3 Number of rationales used by the instructors per frame per task. An increase in number of rationales from the expert frame to the teaching frame is indicated in red. The more rationales have been stated, the darker the table tile. In tasks in which more than one explicit structural feature differed (task 4) and the leaving group ability was discussed (tasks 2, 3, 4) instructors tended to use multiple rationales, *i.e.*, multiple conceptual approaches to underpin their claim

Instructor	Task 1		Task 2		Task 3		Task 4	
	expert frame	teaching frame	expert frame	teaching frame	expert frame	teaching frame	expert frame	teaching frame
Baker	1	1	1	1	1	2	3	3
Bell	1	1	1	2	1	2	2	3
Carter	1	1	2	2	1	2	2	3
Davis	1	1	1	1	3	2	2	2
Franklin	1	1	1	1	2	1	2	2
Jones	1	1	1	2	1	1	2	2
Lewis	1	1	1	2	2	1	3	3
Miller	1	1	1	2	1	3	2	3
Robinson	1	1	1	2	2	2	2	2
Smith	1	1	1	1	1	1	3	3

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9. What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry?

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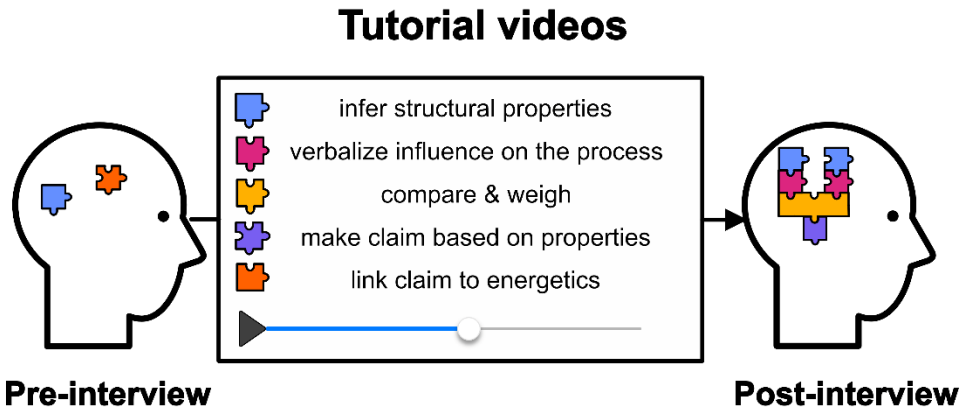

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What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning

Julia Eckhard, Marc Rodemer, Sascha Bernholt, and Nicole Graulich*

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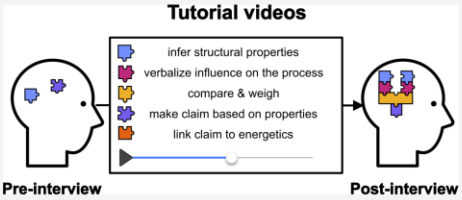
ABSTRACT: Supporting students in building well-grounded explanations plays a crucial role in scientific practice. Research in organic chemistry education on students' mechanistic explanations, however, has revealed various challenges. When solving mechanistic tasks, students experience difficulties when (I) deriving implicit properties from structural formulas, (II) inferring the influence of these properties on the reaction process, (III) comparing and weighing multiple variables, (IV) using structural properties to make a claim, and (V) linking a structural consideration to energetic considerations. Reasoning steps, namely, (I) and (II), can be considered essential for mechanistic explanations, whereas the other steps depend on the task format. One way of supporting learners in these reasoning steps is to provide an instructional explanation that in a guided manner models these steps in tutorial videos. In this study, the design of tutorial videos on substitution reactions, which addresses known students' challenges, is reported. The tutorial videos were put to test in a qualitative pre/post-interview study with students of an undergraduate organic chemistry course (N = 12). While tutorial videos are widely used, little is known about the impact of explicitly designed instructional explanations in videos on students' ability to build mechanistic explanations. Hence, the findings of this study aim to contribute to the growing area of mechanistic reasoning by analyzing how students alter their mechanistic explanations after watching explicitly designed tutorial videos. Differentiated content analysis reveals that students adapt different aspects outlined in the tutorial videos. Overall, students infer more structural properties and use these to make a claim after watching the videos. However, linking this claim to the energetics of a reaction seems to remain challenging. Recommendations for the use in teaching as well as further development possibilities of the videos are presented.



KEYWORDS: *Multimedia-Based Learning, Mechanisms of Reactions, Problem Solving/Decision-Making, Second-Year Undergraduate, Chemical Education Research*

FEATURE: Chemical Education Research

■ INTRODUCTION

Currently, tutorial videos are omnipresent and are recognized as an effective, easily accessible educational tool, e.g., one that is capable of fostering students' engagement with the content through visualizing complex procedures or processes.[1] Prior research on the effectiveness of tutorial videos in general often focused on evaluating the (visual) design, reporting best practice examples or learners' usage and evaluation of the videos, while few studies report in detail how instructional explanations in tutorial videos were derived and what students adapt from these explanations.[2−5]

Students' Prerequisites for Mechanistic Reasoning in Organic Chemistry

In organic chemistry, a large body of research has already elicited students' prerequisites for building mechanistic explanations in organic chemistry. Mechanistic explanations account for *how* and *why* a phenomenon comes about, involving entities with their properties (e.g., molecules or atom groups with their capacity to attract electrons) and their activities (e.g., possibilities to attack as a nucleophile).[6] A mechanistic explanation entails reasoning about multiple variables and their complex interplays to generate cause−effect relations that help to understand, explain, and predict phenomena.[7]

Past studies have shown that students are not able to fully make use of the explanatory power of mechanisms. They encounter various challenges or choose minimalistic ap-

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proaches that contribute little to meaningful learning, such as rote learning[8] or the use of unproductive heuristics.[9] The observed challenges can be attributed to a variety of reasons. Traditional organic chemistry courses, for example, often emphasize product-oriented learning and assessments.[10] Hence, students are not accustomed to developing elaborate explanations for mechanistic tasks.[11] On the basis of the challenges students face, several interventions and curriculum changes have been developed (e.g., changes in curriculum[12,13] or course structure,[14] the implementation of explicit prompting,[15] and scaffolds[16−18]).

To date, little attention has been given to the role of tutorial videos in supporting students' mechanistic explanations in organic chemistry. The focus of this study is thus to determine if and how tutorial videos can support students in building mechanistic explanations.

■ THEORETICAL PERSPECTIVE

Effectiveness of Tutorial Videos

Tutorial videos are regarded as a highly effective educational tool for visualizing (abstract and complex) processes, as video instruction "*adds auditory engagement to visual, language comprehension and cognitive processes, and allows for more varied emphasis of the importance of content*"[19] (ref 19 p. 933). Several studies investigated the effectiveness of tutorial videos in science education,[1] e.g., with regard to fostering students' motivation, interest, and engagement,[19] student satisfaction,[19,20] and achievement.[19−21] Nevertheless, merely watching tutorial videos does not make them inherently effective for learning, as an illusion or overestimation of knowledge acquisition might be promoted.[22,23] To increase effectiveness of videos in terms of learning gains, key elements must be taken into account when designing and implementing tutorial videos in teaching contexts.[1]

Design Principles for Tutorial Videos

For the effective design and implementation of tutorial videos in instruction, several authors defined key elements that need to be considered.[1,2,5] On the basis of the cognitive load theory (CLT) by Sweller (1988),[24] and the cognitive theory of multimedia learning (CTML) by Mayer (2005),[25] learning is bounded to cognitive capacity (cf. refs 1, 24, 25). According to these theories, effective instructional material should facilitate the use of mental resources to support learning, i.e., support cognitive processing of information.[25] Mayer (2021),[2] for example, recently defined evidence-based principles for the design of tutorial videos. These principles regard *reducing of extraneous processing*,[2] i.e., reducing extraneous load by reducing cognitive effort that does not lead to the learning goal. Within this regard, using visual cues (signaling principle) or reduction of irrelevant or distracting aspects to the learner (redundancy principle) is reported to guide their attention to the relevant content. Further principles advise to facilitate the *management of essential processing*,[2] i.e., reducing intrinsic load of the content, by structuring or chunking the content (segmenting). Mayer (2021)[2] further states principles that *foster generative processing*,[2] i.e., enhance germane load, are needed to reach the learning goal. Enhancement of generative processing is linked to key aspects of active learning and student engagement that guide effective design and implementation of videos,[1] for example, using guiding or interactive questions to improve memory and self-assessment or using conversational language (personalization) or brief length of a video are suggested.[1,2]

When regarding the effectiveness of learning videos, multimedia design criteria are often brought to the fore. However, the role of the instructional explanations entailed in such videos is rarely highlighted, although it is crucial, e.g., in terms of how appropriate the content is presented to the learners and perceived by the learners.[5]

From an educational psychology perspective, several criteria need to be considered when constructing instructional explanations (cf. refs 5, 26, 27). Special emphasis is given to the *adaptation to learners' prerequisites*, in terms of interest, alternative conceptions, and prior knowledge, as these influence what learners take away and understand from the videos.[5] According to Kulgemeyer (2018) considering learners' interest might promote motivation to follow the explanation.[27] Furthermore, research in recent decades elicited several alternative conceptions learners have about scientific topics.[28] Within this regard, it has been shown that instructional explanations anticipating them, e.g., by embedding specific hints and prompts, have been useful to overcome these.[29,30] Hence, adaptation to alternative conceptions and content knowledge is considered to foster cognitive activation, i.e., deep processing, and student engagement with the content of the explanation.[27] According to Wittwer and Renkl (2008),[26] who focused on teacher explanations, an instructional explanation ideally addresses diagnosed understanding or prior research on understanding of the targeted viewers. While in a classroom context the adaptation to learners' prerequisites can be achieved through direct teacher−student interaction, an instructional explanation in a tutorial video needs to be carefully adapted to the prerequisites of a target group in advance. The explanation of a video remains the same without a possible in situ adaptation (at least with regard to the video itself, while the interpretation of the explanation and the handling of the video content is certainly influenced by the embedment in the classroom situation). Hence, when comparing instructional explanations in the classroom with instructional explanations in multimedia tools, the importance of carefully considering the target group's prerequisites in advance emerges.

Reasoning Steps and Known Student Prerequisites to Derive an Instructional Explanation in Tutorial Videos

In this study, the instructional explanations in the videos were structured using five key reasoning steps, i.e., (I) inferring structural properties, (II) verbalizing the influence on the reaction process, (III) comparing and weighing structural properties, (IV) making a claim based on structural properties, and (V) linking a structural claim to energetics. These reasoning steps correspond to key aspects of mechanistic reasoning, which are described in the chemistry education literature, e.g., by Sevian and Talanquer (2014),[31] Becker et al. (2015),[32] Cooper et al. (2016),[33] and Caspari et al. (2018).[34] In the following, exemplary empirical findings are shown, which describe researched students' challenges when solving mechanistic problems, to emphasize the relevance of the reasoning steps in the instructional explanation of the videos.

Reasoning Steps I and II: Inferring Structural Properties and Verbalizing Their Influence on the Reaction Process. Considering structure−property relationships and deriving chemical meaning from structural formulas can be considered the key reasoning step for (successfully) applying

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conceptual knowledge, making structure−reactivity judgments, and, accordingly, mechanistic problem-solving. Several studies have shown that students experience problems when decoding representations and inferring chemical concepts and that they focus on the surface features of structural formulas instead of inferring implicit properties when solving mechanistic tasks.[35−39] Hence, an instructional explanation should emphasize how to infer structural properties (reasoning step I). Additionally, students show entity-oriented problem-solving approaches with little consideration of the ongoing reaction process.[40,41] Christian and Talanquer (2012)[42] found, for example, that many students focused on "*representational and structural issues rather than on the more process-oriented aspects of a problem even when working on tasks related to reactivity and reaction mechanism.*"[42] (ref 42 p. 293). Strickland et al. (2010)[40] further found that "*[i]n addition to treating the inscriptions as representations of static entities, the participants rarely, if ever, explicitly spoke of the movement of electrons when describing the mechanisms.*"[40] (ref 40 p. 298). Other studies could report as well that students who engaged in process-oriented problem solving were more successful in solving tasks in organic chemistry[43] or more able to establish causal relationships in mechanistic reasoning (e.g., relating structural changes of a reaction to energetic changes).[44] Hence, describing the interactions of entities and the influence of the structural properties of such entities in the reaction process is a prerequisite for building cause−effect relationships, which should be emphasized in an instructional explanation (reasoning step II).

Reasoning Steps III and IV: Comparing and Weighing Structural Properties and Making Claims Based on Structural Properties. Research on students' approaches to mechanistic tasks further revealed that multivariate reasoning, i.e., weighing different variables, such as the reactivity of functional groups, represents a challenge for students. Furthermore, students' use of case-based reasoning, relying on past (rote-memorized) experiences[42,45] or on one-reason decision-making instead of considering multiple variables, i.e., several structural properties, is documented.[46−48] Bhattacharyya (2014),[49] for example, found that students focused on a "*single parameter*"[49] (ref 49 p. 595) when reasoning about the reactivity/reactive side of a multifunctional molecule. To give students alternative approaches to using heuristics, such as one-reason decision-making, and to promote multivariate thinking, instructions should illustrate the inference of several properties and the weighing of properties (reasoning step III) to make a claim based on structural properties (reasoning step IV).

Reasoning Step V: Linking Structural Considerations to Energetic Considerations. Furthermore, many tasks in organic chemistry concern transformations, e.g., why a certain reaction follows a certain pathway.[50] To appropriately answer these questions, a claim about the energetic course of a reaction is required. To derive such a claim, a structural claim needs to be made first. Goodwin (2003)[50] states that it is required to apply "[...] *robustly applicable concepts that allow one to convert recognizable structural features of the molecules or classes of molecules involved in the question into qualitative energy differences between those entities. These robustly applicable concepts form a bridge between structure and energy.*"[50] (ref 50 p. 144). Studies that researched students' understanding of the relationships between structural considerations and energetic considerations found students struggling in determining causal relationships between implicit properties and potential energy changes[51] and a weak connection when students related such properties to statements about activation energy.[44] To support students in making statements about energy when confronted with chemical transformations, instructions need to explicitly link structure to energy, i.e., inferring energetic considerations (e.g., energetic lowering of the transition state) from structural considerations (e.g., influencing structural properties of functional groups) (reasoning step V).

As all these illustrated reasoning steps for appropriately solving mechanistic tasks are crucial for students to build elaborate explanations, we embedded these steps by "modeling" an instructional explanation in video tutorials. However, little is known about what students actually take away or adopt from these instructional explanations in videos and how they can impact students' reasoning. This report thus includes, on the one hand, the explicit design of tutorial videos on substitution reaction mechanisms by acknowledging the known challenges of students and, on the other hand, seeks to explore the impact of these tutorial videos on students' mechanistic explanations. Qualitative content analysis is used to determine how students alter their mechanistic explanations after watching tutorial videos and to derive possible learning effects and the lack of learning effects.

■ RESEARCH QUESTIONS

This study aims to explore what students learn when watching tutorial videos for organic chemistry and how tutorial videos affect the students' mechanistic explanations. The analysis is concerned with whether and how students adapt the reasoning steps promoted in the videos. We consider the inferences of the structural properties and the verbalization of the influence on the reaction process as the key reasoning steps that are needed to build further reasoning steps, such as comparing and weighing multiple variables, using a structural property to make a claim, and linking a structural claim to energetics. Thus, the following research questions guide our study:

1. How do students infer structural properties and verbalize the influence on the reaction process while explaining case comparisons before and after watching the purposefully designed videos?
2. How are students engaged in further reasoning steps, such as comparing and weighing multiple variables, using a structural property to make a claim, and linking a structural claim to energetics, before and after watching the purposefully designed videos?

■ METHODS

The study reported herein is part of a previously conducted mixed-methods intervention study with purposefully designed tutorial videos. Accompanying pre- and post-interviews were conducted to uncover possible effects of watching tutorial videos on students' mechanistic explanations. The qualitative content analysis of these interviews adds to the quantitative results reported elsewhere[52] and offers an in-depth perspective on students' learning with tutorial videos.

Participants and Setting

The interview study took place at a German university during the summer of 2019 in an undergraduate organic chemistry course (OC I). The lecture followed a rather traditional teaching approach (structured by functional groups, mecha-

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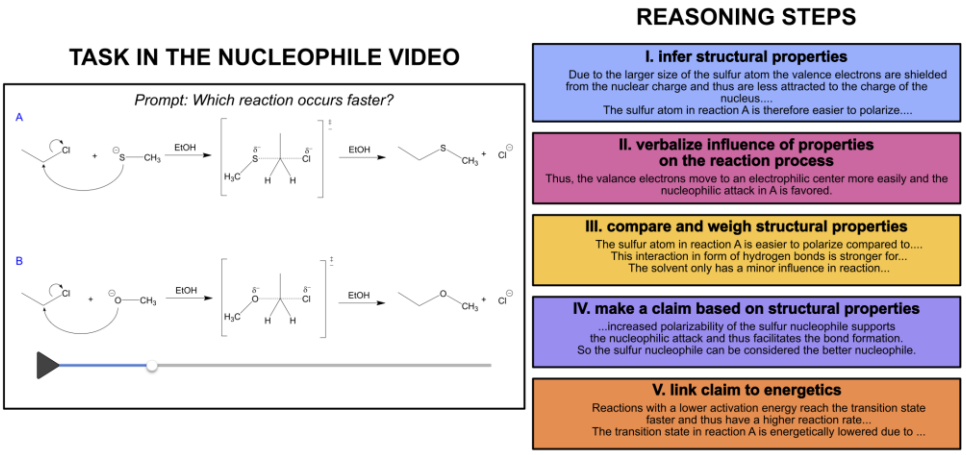

Figure 1. Case comparison task used in the nucleophile video (left). Cases differ in the nature of the nucleophile, and the task prompt was to answer which of the reactions proceeds faster. Reasoning steps and exemplary excerpts of the instructional explanation implemented in the tutorial videos (right).

nism types, and name reactions). The data collection was timed in a way that nucleophilic reaction mechanisms were already covered. Twelve students volunteered to participate in the interview study, i.e., a convenience sample from the students at hand resulted. The research design followed ethical standards in line with the German Research Foundation (IRB approval is not a requirement at German universities), and informed written consent was obtained prior to the data collection. Students were provided with information about the handling of the data and their rights. Moreover, it was explained to them that participation would not affect their course grade and that they could opt out at any time without any consequences. The interviews were conducted in German, and quotes were translated verbatim for this publication. To avoid biases and protect the students' identities, they have been given pseudonyms, which do not reflect their race, gender, ethnicity, or other identities.

Tutorial Videos

The tutorial videos cover nucleophilic reaction mechanisms and the aspects that influence reactivity, leading to three videos, namely, a "substrate video", a "leaving group video", and a "nucleophile video".

As inferring and using multiple variables appears to be challenging for students, the task format of case comparisons is used to support the comparisons of variables. Case comparisons are generally considered a valuable instrument to elicit deeper reasoning (for a meta-analytic review, see ref 53) and have been used to analyze students' construction of mechanistic explanations in organic chemistry.[18,54] In the videos, two cases, reaction A and reaction B, were contrasted by comparing the structural properties and explaining differences in reactivity (Figure 1, left).[55]

The videos were developed regarding the evidence-based principles outlined above (cf. ref 2, 5). To guide learners' attention and reduce extraneous processing, two reactions were displayed, with minimizing further distraction, such as additional text or background color (coherence principle). Furthermore, cues were used (cf. ref 52) to link verbal explanations to the corresponding representations (signaling principle). In order to foster generative processing, e.g., motivation of students, direct addressing was used.[2] Furthermore, a length of approximately 5 min was chosen, as within this amount of time the case comparisons could be explained sufficiently for beginner organic chemistry students. Further, Guo et al. (2014),[56] who performed a large-scale study regarding student engagement, found this length to be effective compared to longer lengths in which the engagement dropped.[56]

To manage essential processing, and support students' engagement with the content, the instructional explanation was structured using reasoning steps (segmenting) and adaptation to students' prerequisites was considered. The structure of the explanations was kept the same across the videos to increase coherence (an exemplary script of an instructional explanation of the videos is available at: https://osf.io/r4sx3/?view_only=84f3319508594da7b1d5d93caf942c3f).

In addition to the conceptual content conveyed, the explanation also emphasizes the approach to solving a case comparison. Each explanation starts with a description of the reaction type, highlighting the occurrence of the transition state. Subsequently, the aim of the case comparison is explained, i.e., to decide which of the two reactions proceeds faster by determining which reaction has a lower activation energy. Here, a necessity to reason about the energetic course of the reaction is highlighted. Then, the overall approach to answer the prompt, i.e., comparing the structural similarities and differences of the two reactions, is mentioned. A general statement about the reaction rate's dependency on breaking the bond between a carbon center and a leaving group and a statement about the bond formation between a nucleophile and an electrophilic carbon atom follows, again aiming at linking structural considerations to the (energetic) course of the reaction.

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After illustrating the reaction type and approach for answering the task prompt, multiple reasoning steps follow as the central element of the explanation (Figure 1, right). Depending on the explicit structural difference shown, different structural properties are inferred (reasoning step I): electronegativity and delocalization in the leaving group video; hyperconjugation, inductive effects, and electronegativity in the substrate video; and electron shielding/polarizability and H-bonding capabilities (capacities to form hydrogen bonds) in the nucleophile video. The structural properties are described with their influence on the reaction process (reasoning step II). Therefore, a process-oriented description of electron movement is used. In further reasoning steps, the structural properties and their influence are used when comparing and weighing structural properties (reasoning step III) and making a claim based on the properties (reasoning step IV). In the last part, the aim of the video is restated, i.e., to decide which of the two reactions proceeds faster by determining which reaction has a lower activation energy. Hence, the structural considerations are linked to energetics when regarding the energetic lowering of the transition state (reasoning step V).

An independent expert in organic chemistry reviewed and approved the explanations. For the original (German) and translated videos, see https://osf.io/r4sx3/?view_only=84f3319508594da7b1d5d93caf942c3f.

Interview Task

For the pre/post-interview, an S_N2 case comparison task was used, as it corresponds to the type of reaction that was covered in the tutorial videos (Figure 2). The reacting molecules of the interview task have similar surface features and properties as the molecules used in the tutorial videos, allowing us to analyze which aspects students incorporate in their mechanistic explanation after watching the videos. A sample solution of the task, approved by an independent expert in organic chemistry, can be found in the Supporting Information (Table S1).

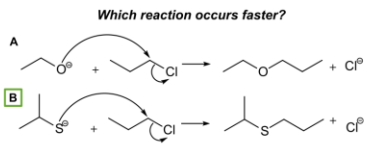

Figure 2. Case comparison task used in the pre- and post-interviews (correct answer is highlighted—however, it was not highlighted for the students in the interview).

DATA COLLECTION

Pre-interviews were conducted in person in the week before the intervention, i.e., up to 4 days before watching the tutorial videos, and post-interviews were conducted in the week after watching the videos.

During the semistructured in-person interviews, a student sat together at a table with the interviewer and was shown the interview case comparison task on a sheet of paper. The students were video- and audio-recorded while they completed the task (the task remained the same pre and post) (Figure 2). Students were asked to think-aloud when explaining, and the interviewer asked clarification questions to reassure the understanding of the intended meaning (for an excerpt of the semistructured interview protocol, see Supporting Information, Table S2). During the intervention, students watched tutorial videos on laptops or tablets. In the post-interview, specific questions were asked whether students changed their approach to solving the task.

DATA ANALYSIS

The interviews were transcribed verbatim and implemented into the coding software MAXQDA for qualitative content analysis. Data analysis began with an initial review of the data by reading the transcripts multiple times, taking notes, and creating case summaries per student.[58] Since we were interested in what students were learning from the videos, a deductive coding system was developed, structured by the five reasoning steps implemented in the videos (Supporting Information, Table S3) to afford a reliable inference of students' assumptions.[57] The first category, "(I) inferring structural properties", entails the use of subcodes representing the structural properties, i.e., electronegativity, polarizability, inductive effects, and steric hindrance, that were covered in the tutorial videos and relevant to the task solution. The codes were assigned if the students named the structural property and the chemical concept or described it in their own words. Furthermore, the category "(II) verbalizing the influence on the reaction process" covers whether a student described how a structural property affects the course of the reaction, e.g., if a property leads to facilitated bond breaking or bond formation.

The category "(III) comparing and weighing of structural properties" characterizes how students balanced several properties (e.g., comparing inductive effects and polarizability or weighing electronegativity against polarizability). The category "(IV) making a claim based on a structural property/several structural properties" captures students' decision-making, aiming at characterizing the students' approach to supporting their claims compared to other approaches, such as gut feeling or heuristics. The fifth category "(V) linking structural claim to energetics" characterized whether a student refers to energy and thus establishes a link between structural considerations and the energetic course of the reaction, e.g., if structural claims are related to activation energy or the energetic lowering of the transition state.

During the development, the coding system and coding units were discussed between all authors. Two members of the research team then applied the initial coding system on a trial basis. The whole research team adjudicated coding disagreements until complete consensus was reached.[59,60] Hence, to ensure that coding decisions faithfully represented the data and to reach high intercoder agreement, the coding system was revised; i.e., the codes and their definitions were refined to their current state. For interrater reliability, two members of the research team coded a random sample of 20% of the data independently. A chance-corrected Kappa coefficient[61] of 0.92 was calculated, indicating high agreement and reliability.[62,63] Then, the first author coded the remaining data.

RESULTS AND DISCUSSION

In the following, the findings are structured and discussed according to our research questions. The quotes presented are selected excerpts from longer passages of the interviews that provide illustrative evidence to support the results.

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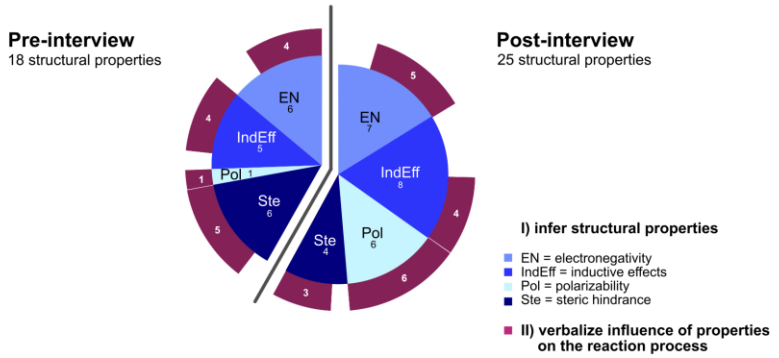

Figure 3. Pie chart representing the results of inferred properties in the pre-interview (left) and in the post-interview (right). The inner ring shows the distribution of the mentioned structural properties (shades of blue). The outer ring (raspberry colored) shows by its width how often the influence of a property of the inner ring was verbalized on the reaction process.

RQ1: How Do Students Infer Structural Properties and Verbalize the Influence on the Reaction Process while Explaining Case Comparisons before and after Watching the Purposefully Designed Videos?

Students Show an Increased Use of Structural Properties after Watching the Videos. A content analysis of students' explanations of the interview task revealed that the inference of structural properties increased from before to after watching the videos (Figure 3). Thereby, 12 students verbalized 18 structural properties in the pre-interview and 25 structural properties in the post-interview. In the pre-interview, the considered properties were mostly electronegativity (n = 6), steric hindrance (n = 6), and inductive effects (n = 5), whereas polarizability (n = 1) was referenced once. In the post-interview, the distribution of inferred structural properties changed. Structural properties inferred in the pre-interview were used again, and new properties were mentioned. After watching the videos, derived properties were mainly inductive effects (n = 8), electronegativity (n = 7), and polarizability (n = 6), while less was argued about steric hindrance (n = 4) (cf. Figure 3).

Before watching the videos, 8 out of 12 students were thus able to infer structural properties from the structural formulas. The remaining four students could not decide or relied on explicit surface features, such as "*better looking nucleophile*", or gut feeling to make their claim. The students who inferred structural properties in the pre-interview often chose the higher electronegativity of oxygen compared to sulfur or/and a statement about steric hindrance as a basis for their argumentation and thereby neglected the differences in polarizability. The fact that students rely on steric hindrance in solving case comparisons is in line with prior research and indicates that students find it easier to use accessible explicit features, such as the size of the structural formulas of the nucleophiles, in their rationales instead of inferring implicit electronic properties, such as electron shielding and polarizability.[18,54]

In the post-interview, all students succeeded in deriving structural properties and used them in their further line of reasoning. They thereby additionally included polarizability and a consideration of inductive effects within the nucleophiles. Hence, this increase is particularly noteworthy, as these properties were mentioned in the nucleophile video, indicating that the tutorial videos supported students in including these aspects in their reasoning.

The findings show that students verbalized the influence of a structural property on the reaction process comparably often in the pre- and post-interviews, e.g., describing how a property leads to a facilitated nucleophilic attack on the electrophilic center (Figure 3, outer ring, raspberry color; pre: 14 out of 18 properties and post: 18 out of 25 properties were verbalized with an explicit description of the influence on the reaction process). Notably, the structural properties not mentioned in the pre-interviews but inferred in the post-interviews were often related to the reaction process. This indicates that the newly derived concepts were not only mentioned as "empty envelopes" but were also verbalized in a process-oriented manner and that students constructed meaning from the given information in the tutorial videos. To exemplify these findings, one can compare Isaac's statements of the pre- and post-interviews (Figure 4).

In the pre-interview, Isaac inferred inductive effects and electronegativity. He stated that he relied mainly on inductive effects of the alkyl backbone in addition to differences in electronegativity between sulfur and oxygen to determine which entity is more stable. In this statement, he did not refer to the nucleophilic capacities and the process of the reaction. He focused on determining the stability of the products to make a decision regarding a faster reaction, which is in line with prior research showing that students often focus on products, i.e., using static approaches to describe change.[18,44] In the post-interview, he additionally referred to the polarizability of the heteroatoms and hence inferred an additional structural property. He addressed the different sizes of the heteroatoms, deducing that this leads to differences in polarizability, which leads to an increased attraction of the sulfur nucleophile to the electrophilic center ("*the more polarized it gets and the more strongly it is attracted*"). After watching the videos, Isaac thus complemented his pre-interview thoughts with an additional property, which he related to the reaction process. He further referred to the electronic structure ("*the outer electrons can be distributed*

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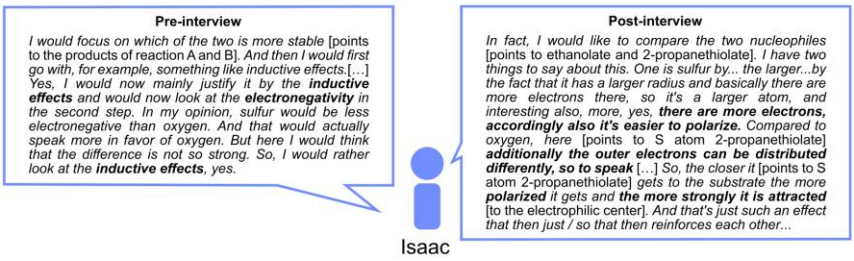

Figure 4. Isaac's statements of the pre- and post-interviews representing how he inferred structural properties (reasoning step I + II).

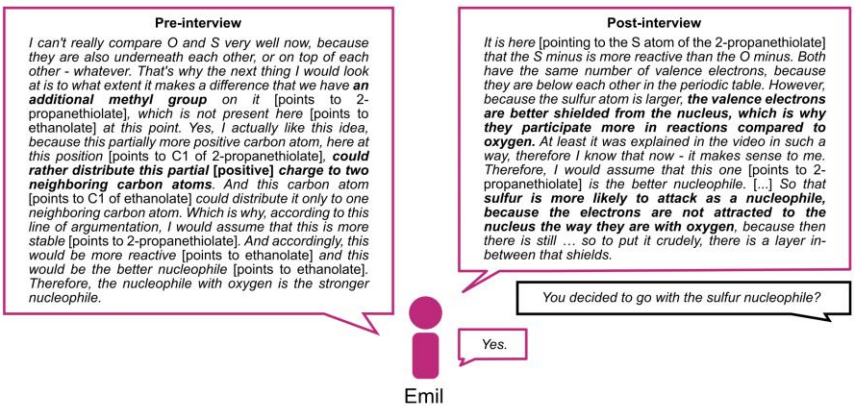

Figure 5. Emil's pre- and post-interview statements representing how he inferred structural properties and the influence on the reaction process (reasoning step I + II).

differently"), which he did not mention in the pre-interview. As Isaac's explanation points out, students are often able to infer more structural properties after watching the videos, especially adding polarizability to their reasoning. Another example that underlines how students changed their inference of structural properties after watching the videos is illustrated with Emil's statements (Figure 5).

In the pre-interview, Emil could not derive any implicit properties from the difference of the heteroatoms, since he could not distinguish "*O*" and "*S*", as they are "*underneath each other*" in the periodic table of elements. Therefore, he used the different number of alkyl groups and inferred the charge-distributing capacities of the methyl groups as a basis for argumentation.

He described the stabilization of the "*partial* [positive] *charge*" via the distribution to the neighboring methyl groups, which—in his eyes—leads to a reduced reactivity of the sulfur nucleophile. The shape of the backbone of the sulfur nucleophile reminded him of tertiary carbocations. However, the inductive effects of the methyl groups exhibit an electron push toward the heteroatom, increasing the nucleophilicity of the sulfur nucleophile compared to the oxygen nucleophile. He neglected the properties of the heteroatoms and reasoned about the stability of carbocations (on which the backbones of the nucleophile reminded him). In the post-interview, Emil succeeded in deriving a structural property from the heteroatoms, which he attempted to do in the pre-interview. Hence, he was able to distinguish "*O*" and "*S*" and reasoned about electron shielding.

Emil's statement exemplifies how the structural property of polarizability was inferred, which can be attributed to tutorial videos ("*...it was explained in the video in such a way.*"). Emil further verbalized the influence of the newly inferred property on the reaction process; i.e., "*So that sulfur is more likely to attack as a nucleophile because the electrons are not attracted to the nucleus the way they are with oxygen*".

Taken together, the findings suggest that students are encouraged to derive more properties after watching the videos, especially of the heteroatoms of the nucleophiles, which can be related to their being engaged with tutorial videos. In general, it is shown that—in addition to new properties—students also relied on properties they mentioned in the pre-interviews and verbalized them with an influence on the reaction process. This could serve as an indicator that the videos were able to tie in with the students' prior knowledge and added to their knowledge, which has been suggested to be meaningful from an instructional perspective.[26] At this point, however, in learning, care must be taken when concepts of prior knowledge are applied in an incorrect context (as shown in Emil's explanation in the pre-interview). Students further

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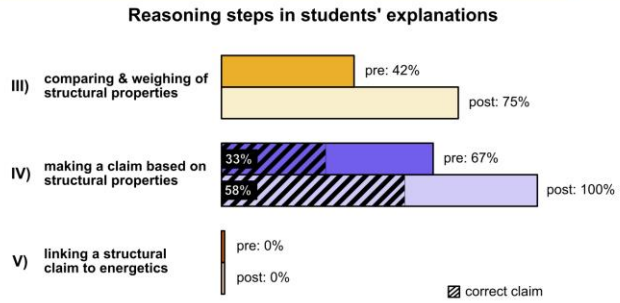

Figure 6. Reasoning steps in students' (N = 12) explanations before (pre) and after (post) watching the videos. Yellow bars: reasoning step "(III) comparing and weighing structural properties". Purple bars: reasoning step "(IV) making a claim based on a structural property/several structural properties" (before watching the videos a third of the students did not make a claim, another third stated correct claims (indicated by the shaded areas), whereas the other third stated incorrect claims; in the post-interview: 58% of the claims were correct (indicated by the shaded areas)). Orange bars: reasoning step "(V) linking a structural claim to energetics".

often verbalized the influence on the reaction process and made less use of entity-oriented approaches to determine which nucleophile is "*more stable*". Moreover, verbalization of the change provided more references to the electronic structure and electron movement after watching the videos. This can be observed in Isaac's description of the polarizability of the sulfur atom ("*there are more electrons, accordingly also it's easier to polarize*") or Emil's description of loosely held electrons in the sulfur atom ("*sulfur is more likely to attack as a nucleophile, because the electrons are not attracted to the nucleus the way they are with oxygen*").

In cases in which the influence on the reaction process was not verbalized, students might oversee the necessity to express this step or find it challenging to relate properties to the reaction process. The latter was also found in previous studies, showing that verbalizing an influence of an implicit electronic property is especially demanding, as this completion of a cause−effect relation in an explanation represents an increased complexity with a higher level of abstractness.[44] Furthermore, students did not tend to verbalize the influence on the reaction process for every mentioned property individually. This was especially evident in the post-interviews when students were able to derive multiple properties. This may hinder the formation of a well-grounded claim in further reasoning steps, since derived properties and their influences could point in different directions when comparing and weighing them.

Overall, the videos advanced students' conceptual understanding by supporting them in inferring (multiple) structural properties and using properties in their reasoning.

RQ2: How Are Students Engaged in Further Reasoning Steps, such as Comparing and Weighing Multiple Variables, Using a Structural Property to Make a Claim, and Linking a Structural Claim to Energetics before and after Watching the Purposefully Designed Videos?

The second research question addresses how students are engaged in further reasoning steps using structural properties to approach case comparison tasks (Figure 6). As shown in Figure 6, the use of reasoning steps "(III) comparing and weighing structural properties" and "(IV) making a claim based on structural properties" increased, whereas reasoning step "(V) linking a structural claim to energetics" was not mentioned before and after; hence, no change could be observed.

Compare and Weigh Structural Properties. Before watching the videos, in the pre-interviews, students often relied on one variable or on recognition of a memorized reactivity order. After watching the videos, they more often succeeded in comparing and weighing multiple variables, i.e., structural properties (Figure 6, pre: 42%; post: 75%). As this reasoning step is related to the number of structural properties mentioned, it is not surprising that after watching the videos—when more structural properties were inferred—structural properties were also increasingly compared and weighed. Amy's responses to the interview task provide an example (Figure 7).

In the pre-interview, Amy inferred the property of electronegativity of oxygen and did not weigh further structural properties. She described an influence of the property, namely, a greater ability to pull electrons leads to a higher capacity of the oxygen nucleophile to attack the partial positive charge. When asked about the impact of that influence on the reaction, she said that the reaction with the oxygen nucleophile would be faster. In the pre-interview, she did not compare and weigh multiple structural properties in her line of reasoning and focused on one variable, an approach that was also found in previous studies.[42,47,49] Although she has drawn on this property of the oxygen atom, she based her decision on her gut feeling and chose the reaction with the sulfur nucleophile to be the faster one. In the post-interview, in contrast to the pre-interview, she considered a property of the carbon backbones of the nucleophiles in addition to the electronegativity of the heteroatoms; i.e., she used two structural properties. Amy argued that the oxygen atom has an increased electronegativity, which would lead her to prefer the reaction with the oxygen nucleophile. She thereby showed the same explanatory approach as in the pre-interview. In addition, she thought about the impact of the increased number of alkyl groups attached to the sulfur nucleophile. Ultimately, she concluded that this leads to an increased charge of the sulfur nucleophile due to electron donation toward the sulfur atom. Compared to the rationale she used in the pre-interview, the rationale Amy used in the post-interview included an additional property. Her attempt at weighing the properties

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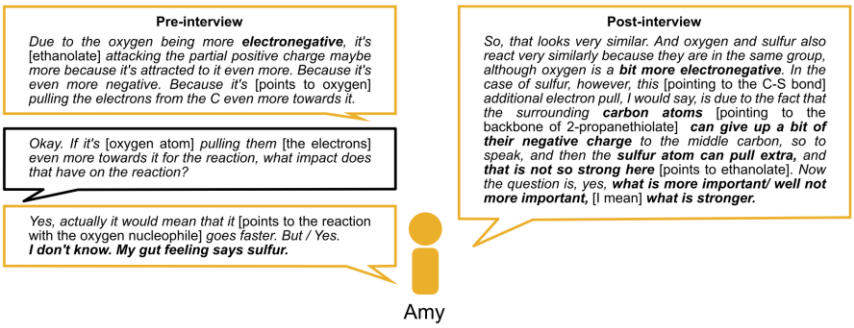

Figure 7. Amy's pre- and post-interview statements representing how she compared and weighed structural properties (reasoning step III).

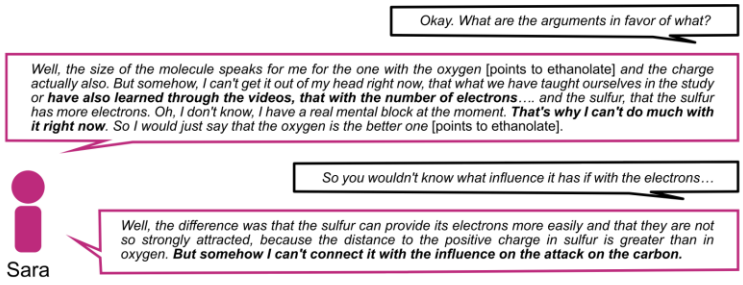

Figure 8. Sara's statement in the post-interview showing how she struggled to compare and weigh structural properties, i.e., include properties of sulfur in her reasoning, as she is not aware of the influence on the reaction process ("*I can't connect it with the influence on the attack on the carbon*").

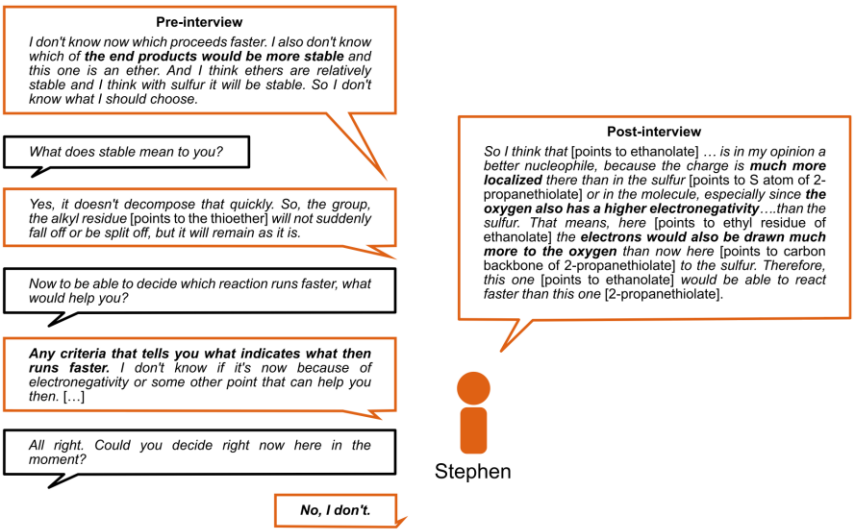

Figure 9. Stephen's statements showing how he was not able to make a claim in the pre-interview (left) and how he made a structural claim considering electronegativity as a structural property after watching the videos in the post-interview (right) (reasoning step IV).

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is especially evident at the end of the statement. She showed that comparing and weighing the properties and their influences was not easy for her and wondered what was "*more important*" or "*stronger*", weighing higher electronegativity against inductive effects, i.e., the "*charge donation*" of surrounding carbon atoms. Hence, the way Amy reasoned changed after watching the videos, i.e., from a gut feeling decision in the pre-interview to a more structured approach including the weighing of multiple properties after watching the videos in the post-interview.

The findings of students struggling to weigh several properties are in line with findings by Watts et al. (2021).[18] Their findings showed that even with the use of a tool such as a scaffold, students did not always weigh several variables and showed uncertainty in how to balance properties.[18] This confirms that the reasoning step of comparing and weighing is a challenging step for students and needs support in teaching.

The findings further revealed that it was easier for the students to compare and weigh the properties if the influence on the reaction process was inferred by the students in their reasoning. This can be exemplified by Sara's statement (Figure 8). In the post-interview, Sara was able to infer polarizability as an additional property, which she verbalized electronically ("*sulfur can provide its electrons more easily and they are not so strongly attracted, because the distance to the positive charge in sulfur is greater than in oxygen*"). However, Sara struggled to verbalize an influence on the reaction process (Figure 8). She could not match this statement with the attack on the electrophilic center and identified a gap in her reasoning.

Sara was aware that the influence of an increased number of electrons was conveyed in the videos but stated she had a "*mental block*" as to why she was not able to "*do*" anything with the property in the interview task. She struggled and ultimately relied on other properties whose influence on the reaction process was more familiar to her. The struggle led her to experience problems in comparing and weighing multiple variables and highlights that an important prerequisite for this step and ultimately for decision-making is the derivation of multiple structural properties as well as the awareness of their influence on the reaction process.

Make Claims Based on Structural Properties. After watching the videos, there was an increase in the category "making a claim based on a structural property" (Figure 6, pre: 67%; post: 100%). In the post-interview, all students stated a final claim after inferring one or several structural properties. This is noteworthy because a commonly reported challenge is decision finding. Students often tend to make claims based on explicit features instead of on implicit features and make use of heuristics (such as recognizing reactivity orders taught in the lecture), or gut decisions.

Stephen's task solution exemplifies how the use of structural properties enabled him to make a claim in the post-interview (Figure 9).

In the pre-interview, he was not able to derive and use structural properties to make a claim. In his reasoning, he focused on the "stability" of the products to make a claim, which is in line with students' reasoning found in prior studies.[34,54] However, he was not able to attribute a higher stability to a certain product and make a claim based on structural properties. Stephen did not elaborate on structural properties and the source from which this stability results (even when prompted later in the interview) and stated the need for "*criteria*", i.e., structural properties, such as differences in electronegativity, to be able to make a claim. Hence, he did not state a claim based on structural properties.

In the post-interview, Stephen succeeded in inferring a structural property, i.e., electronegativity, and claimed that the reaction with the oxygen nucleophile was faster. Even though Stephen stated a wrong claim, he was able to apply a "criterion", i.e., electronegativity, and contrast the reactions. One could relate his inference of this structural property in the post-interview to his having learned this concept in the leaving group video in which electronegativity properties were entailed. One indicator is shown by his verbalization of electron movement associated with electronegativity and the charge localization ("*charge is much more localized*"), aspects that were emphasized in the videos.

After watching the videos, claims were more often correct (Figure 6, pre: 4 out of 12 students stated correct claims; post: 7 out of 12 students stated correct claims) and were often stated including the structural properties of polarizability and the inductive effects. Students who stated wrong claims in the post-interview often relied on a single property. In particular, the electronegativity of the oxygen atom was an accessible concept for them pre and post (Figure 3), presumably because it is frequently used as an example in lectures (e.g., regarding carbonyl chemistry). Further, students who stated wrong claims often neglected structural properties (especially polarizability of the sulfur nucleophile) and did not compare and weigh several properties, as Stephen's example illustrates (Figure 9, right). The outcome of the reasoning step, i.e., correct/incorrect claim, hence, is not independent from previous reasoning steps, such as inferring structural properties. Moreover, students stating wrong claims can be related to short-term learning effects, as well as the fact that the interview task was more demanding than the task in the nucleophile video, as it required multivariate reasoning due to multiple structural differences.

Note that while in the pre-interview, correct claims were often based on heuristics, such as relying on memorized reactivity orders (and there may have been little substantive understanding behind the claims), in the post-interview, correct claims were often made based on several structural properties and their weighing. This finding further emphasizes that when assessing mechanistic reasoning, not only the final claim but also the students' approaches to solving mechanistic tasks should be assessed.[10]

Link Structural Claim to Energetics. Before and after watching the videos, no links between structural claims and energetics were made in the interviews (Figure 6). This means that students did not include reasoning about the energetic course of the reaction and its relation to structural properties. Thus, no changes can be observed in this reasoning step. Even if one might think that reasoning about "stability" is related to reasoning about energetics, when asked to clarify the meaning, students were not relating their assumptions to potential energy or the energetic proceeding of the reaction; rather, they used the word as a verbalism or related it to structural stability (see Stephen's task solution to the pre-interview, Figure 9).

However, in the post-interview, students showed an awareness that a reference to energetics was conveyed in the videos and needed to be included when solving a case comparison. When students were asked if anything was new to them in the video, the relation to energy mentioned in the videos was often referenced, which can be seen in Amy's statement in the post-interview (Figure 10).

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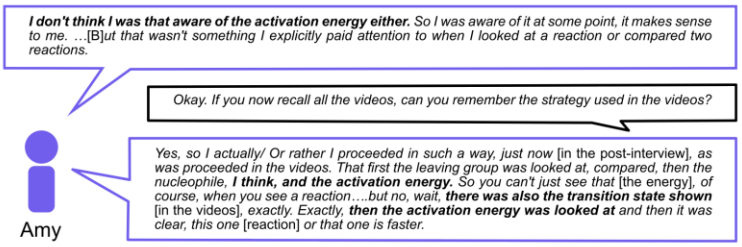

Figure 10. Amy's statements showing that she was aware that reasoning about energy was part of the approach to solve a task in the videos.

Like Amy, most of the students mentioned being aware that energetic claims were made in the videos but did not show this reasoning step in their explanation of the interview task. For example, Isaac explained why he did not consider energetics: "*But the thing with the speed and the activation energy, how that is connected* [...] *I am not quite aware of this causality yet.*" Hence, understanding the causality and verbalizing this step is demanding for students.

The fact that, compared to the other steps, this reasoning step was not included in the mechanistic explanations could be due to various reasons. The students' attention span may have been exceeded since the claim about the energetic course was stated at of the end of each video. Also, the link between structural influences and the energetic course might not have been sufficiently explicit for the students in the instructional explanation. Further, it could be that the step is generally difficult for the students. This is evident in prior research, in which students' challenges in linking structural assumptions to energetics, i.e., reasoning about rate-determining steps, were observed (e.g., refs 44, 51, 54, 64, 65). Challenges in establishing a link between structure and energetics could be because it is not explicitly emphasized in teaching, e.g., because the energy concept is often regarded as prior knowledge.[51]

■ CONCLUSION AND IMPLICATIONS FOR FUTURE WORK

The Videos Support Students in Using Structural Properties in Reasoning Steps and Promote a Structured Approach to Solving Case Comparison Tasks

The qualitative analysis uncovered possible effects and a lack of effects of tutorial videos with regard to changes in students' mechanistic explanations. The findings show that after watching the videos, students were able to infer more structural properties and often made use of them in further reasoning steps, e.g., comparing and weighing several structural properties, to explain a mechanistic task.

After watching the videos, students more often used structural properties conveyed in the videos, e.g., the concept of polarizability. Instead of a buzzword-like naming of structural properties, students often elaborated on what the structural properties implied on a submicroscopic level and included the electronic structure and electron movement in their explanation in the post-interviews. Comparing pre- and post-explanations further showed that the influence of structural properties on the reaction process was verbalized to a comparable amount. The supposed lack of an expected increase within this reasoning step might be because after watching the videos, when students were able to infer more structural properties, the influence on the reaction process was not considered necessary to be verbalized individually for each property.

Our analysis of how students were engaged in further reasoning steps (research question 2) showed an increase in comparing and weighing multiple structural properties. This finding indicates that tutorial videos can support students in multivariate thinking. When engaging in the reasoning step of comparing and weighing, students have difficulties deciding which one of the properties influencing the reaction process predominates. It seems challenging for students to determine the relative strength of the influences, e.g., determining whether inductive effects outweigh potential steric hindrance. Moreover, the results revealed that after watching the videos, all students made a claim based on one or several structural properties. The implementation of this reasoning step into their explanations underlines that students had changed their approach to solve a case comparison, moving away from grounding their claim on surface features or gut feeling. However, the findings reveal that the videos do not further support the linkage between structural considerations and the energetics of a reaction. Statements in the post-interview thus indicated that students were often aware that this step is part of solving a case comparison, but they did not verbalize this step themselves when solving a case comparison on their own.

The large quantitative study associated with this study revealed learning gains in conceptual knowledge from the pre- to the post-test[52] and could show that students with low prior knowledge seem to especially benefit from the videos.

The qualitative content analysis reported herein added a more in-depth perspective on how students are learning with the videos. However, it remains open whether students with a high level of prior knowledge are more likely to adapt the reasoning steps and are able to use them in new contexts after watching the videos, while students with a lower level of prior knowledge are more likely to focus on the declarative information conveyed in the videos, e.g., are able to repeat key terms. Within this regard, Kulgemeyer (2020),[5] reported that instructional videos might primarily foster declarative knowledge, whereas the transferrable, conceptual knowledge benefits from additional instruction, i.e., using learning tasks that ask for the application of the principles explained in the videos to new contexts to foster active learning.[5] Hence, the impact of tutorial videos on students' learning could be further investigated with a focus on how prior knowledge and adapted instruction affects learning with these videos.

Additional tutorial videos could be designed to target individual needs, e.g., videos that highlight specific reasoning steps, e.g., how a structural property is derived, how to assess

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the strength of properties, or how to link structural considerations to energetic considerations.

Future research in this area should further acknowledge the differences between learners, in addition to aspects of prior knowledge differences. Modifying and providing differently designed videos, e.g., built-in subtitles or a picture/mechanism description, might increase inclusivity and accessibility.

■ LIMITATIONS

A limitation of the study is the representativity of the convenience sample. Due to the small sample size (N = 12), findings only allow a limited generalization and the power to identify differences among subgroups (e.g., regarding prior knowledge groups) is lacking. However, the analysis showed that the interviewed students used approaches like recognition of superficial features, rote memorization, and use of unproductive heuristics in the pre-interview—strategies that were characterized in chemistry education research studies before (e.g., ref 39). Hence, the sample represented typical beginner organic chemistry students and the analysis identified (exemplary) changes in students' strategies within the sample. The findings of the present study thus need to be reproduced with a larger student cohort. Furthermore, students' voluntary participation might contribute to self-selection bias, and thus findings are only generalizable to a certain extent. Moreover, the results of the study may be influenced by a novelty effect, as the implementation of the videos represented a special situation to the students that potentially influenced learning. The study was conducted within a two-week period so that the post-interview was conducted in the week after watching the videos. Accordingly, the results only represent short-term learning effects. Further, the time span between the interviews and watching the videos has varied for the participants within a few days. However, the latter was not noticeably reflected in the data, as the participants indicated that they remembered the videos well in the post-interview evaluations. Another limitation is the number of interview tasks and the (surface) similarity of the interview task to the video. The participants could apply similar concepts of the heteroatoms in the interview tasks, which were discussed in the nucleophile video. In this regard, the task can be regarded as a reproduction task. Nevertheless, the interview task also contained elements that require transfer, as two structural differences (different heteroatoms and different backbones of the nucleophiles) instead of one were entailed in the task. Hence, compared to the task in the nucleophile video, participants were required to apply concepts related to (differences in) the backbones of the nucleophile (donating effects of alkyl groups/steric hindrance), which were discussed in the substrate video. For future work, other tasks regarding influential factors of a nucleophilic substitution reaction could add value to the validity of the results. Furthermore, students' verbalizations during the interviews may not always correspond to their reasoning, i.e., the statements could imply deeper meaning. In the interview process, however, this was attempted to be ruled out by reassuring understanding.

■ IMPLICATIONS FOR PRACTICE

The tutorial videos discussed here were targeted at students in undergraduate courses in organic chemistry with a basic understanding of reaction mechanism. Thus, these tutorial videos are appropriate when highlighting the influencing factors of a nucleophilic reaction (nucleophilicity, leaving group quality, substrate effects), as the videos highlight how and which properties can be derived from the structural formulas and weighed. From our results, it became evident that the videos mediate a meaningful approach to solve a mechanistic task and allow students to advance their own mechanistic explanations and to overcome the use of heuristics and simple recall.

How the videos are embedded in instruction may play an important role in facilitating learning from the videos, as a mere watching of videos itself puts students in a rather passive "consuming" position. Even when students watch tutorial videos once, as in the study, learning already seems to be evident (in the short term) conceptually and in terms of adopting the approach. In an instructional setting, segmenting the problem-solving process and reflecting about the reasoning steps might help students recognize the different steps and affordances. Furthermore, students could be asked to attend to the concepts conveyed by being prompted as follows: "*Which structural properties are derived within the tutorial videos*? *How do these properties influence the reactions*?" On the basis of the findings, it became clear that students often do not verbalize an influence on the reaction process for each property individually, although this plays a crucial role in the subsequent weighing step. At this point, an implication for teaching emerges, calling for addressing and practicing the verbalization of the influence of a structural property on the course of a reaction, in addition to deriving (multiple) structural properties.

When using the videos, students could further be prompted upfront to focus on the approach to solve a case comparison, e.g., to explain the following: "*Which sub-steps are to be made when solving a case comparison*?" This could help students recognize the different reasoning steps conveyed in the videos. If practicing and reflecting on the problem-solving process is targeted, the tutorial videos could be used similarly to the study setup, i.e., framed by learning tasks before and after watching the videos. Using follow-up learning activities, such as learning tasks (and reflecting upon one's own used approaches), increases the effective use of explanation videos, as students are engaged in applying newly learned content.[5]

Furthermore, our results showed that support is needed when weighing multiple variables. In addition to the videos, a scaffold could be used, which specifically asks to derive multiple properties with their influences on the reaction process and that supports noticing and balancing different variables.[16] Watts and colleagues (2021)[18] found positive influences of such a scaffold, stating that students' ability to weigh multiple variables increased over time.

Our study showed that students use "stability" as an anchor to determine which reaction proceeds faster. Thus, in the classroom, the link between structural and energetic changes within the course of a reaction could be strengthened; e.g., a concrete meaning should be given to the term "stability" (thermodynamic or kinetic interpretation). Furthermore, "stability" could be used as a connector to bridge structure and energy, and the "stability of products", i.e., the thermodynamic stability, could be related to the activation energy and the reaction rate.

Taken together, the differentiated content analysis revealed how students adapted different aspects outlined in the tutorial videos, i.e., indicating gains in conceptual knowledge and procedural knowledge after watching the videos. Students were

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able to infer more structural properties and use these to make reasoned claims in a mechanistic task, i.e., to perform essential reasoning steps when problem solving. Hence, the tutorial videos can be considered a suitable digital learning tool contributing to students' mechanistic reasoning.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.2c00076.

Sample solution to the interview task; Excerpt of the semistructured interview-protocol; Coding system to identify reasoning steps in students' explanations (PDF)

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Notes

The authors declare no competing financial interest.

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Supporting Information

What Do University Students Truly Learn When Watching Tutorial Videos in Organic Chemistry? An Exploratory Study Focusing on Mechanistic Reasoning

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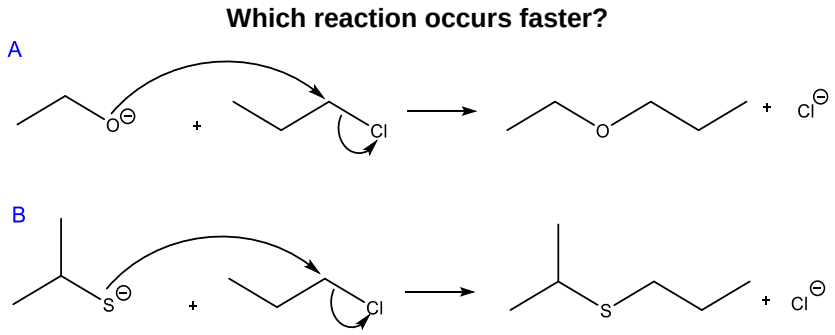
9.1. Supporting Information 1: Sample Solution to the Interview Task.

Table S1. Sample solution to the interview task.

Sample solution to the interview task	
	
Description of the course of the reaction	In each of the reactions shown, a second order nucleophilic substitution occurs. In reaction A, an oxygen nucleophile attacks an electrophilic carbon center. In reaction B, a sulfur nucleophile attacks an electrophilic carbon center. At the same time, a chloride ion leaves the molecules. An ether in reaction A and a thioether in reaction B are formed as products together with a negatively charged chloride ion. Both reactions proceed via a pentacoordinated transition state.
Goal	We now have to decide which of the two reactions occurs faster. Reactions with a lower activation energy reach the transition state faster and thus have a higher reaction rate.
Similarities and differences	To make a decision, we have to compare the similarities and differences of the two reactions. In both reactants, the leaving group, the chloride ion, is identical. One structural difference between the reactions is the heteroatom of the nucleophile. In reaction A, a negatively charged ethanolate ion with oxygen as a heteroatom attacks the electrophilic center, while in reaction B, the negatively charged (1-methyl)ethylthiolate ion with sulfur as a heteroatom attacks the electrophilic center. Another structural difference between the reactions is the backbone of the nucleophiles. In reaction A, the nucleophile entails a (unbranched) two-carbon alkyl substituent, an ethyl group. In reaction B, the nucleophile entails a (branched) three-carbon alkyl substituent, an isopropyl group.
Reference to reaction rate: bond formation and bond breaking	In S_N2 reactions, the reaction rate depends on two factors, namely, the heterolytic breaking of the bond between the carbon center and the leaving group and the bond formation between the nucleophile and the electrophilic carbon atom. Since the leaving groups are identical in both cases, they influence the reaction similarly. Therefore, we only consider the bond formation between the nucleophile and the electrophilic carbon atom. This bond formation depends on how well the nucleophilic attack on the electrophilic carbon center can take place.

Reasoning steps	
I) Inferring of structural properties: electron shielding/polarizability & II) Verbalizing the influence on the reaction process	Concerning the differences of the heteroatoms, as known from the periodic table, sulfur is listed underneath oxygen. Due to the larger size of the sulfur atom, the valence electrons are shielded from the nuclear charge and thus are less attracted to the charge of the nucleus. Thus, they are able to move to an electrophilic center more easily. The oxygen atom in reaction B is smaller, resulting in a higher attraction of valence electrons to the charge of the nucleus. For this reason, the donation of the oxygen's electrons to form a bond is more difficult, i.e., associated with higher energy input. The sulfur atom in reaction B is easier to polarize and due to its significantly lower electronegativity than the oxygen atom in the upper nucleophile, it is better able to share electron pairs with a bonding partner, and the nucleophilic attack in B is favored.
I) Inferring of structural properties: steric hindrance & II) Verbalizing the influence on the reaction process	Looking at the differences of the backbone of the nucleophile, consider the following: In the lower case, the molecular structure of the nucleophile is more branched compared to that of the upper nucleophile. Hence, steric properties need to be considered. Repulsive interactions between the nucleophile and the electrophile take place in terms of electrons repelling each other—especially with the $\sigma_{C\text{-}H}$ orbitals of the CH_2-group adjacent to the electrophilic center and the n orbitals of the nucleophile. In reaction A, the nucleophile is only minimally hindered due to its unbranched backbone, i.e., its electronic structure. Hence, an approaching of the nucleophile in A to the electrophilic center can occur easily. In the lower case, the molecular structure of the nucleophile is more branched. Increased repulsive interactions between the nucleophile and the electrophile take place. However, the C-S bond is longer than the C-O bond. The impairing additional methyl group of the backbone of the nucleophile in B is in a distance when the transition state is formed, whereby the electronic repulsions don't occur so strongly.
I) Inferring of structural properties: inductive effects & II) Verbalizing the influence on the reaction process	Furthermore, the alkyl groups of the nucleophiles donate electron density of their σ-orbitals toward the nucleophilic center due to inductive effects. Due to the additional alkyl group of the nucleophile in B and accordingly the additional electron push, from the perspective of electron density, the nucleophilic attack in B is facilitated in comparison to that in A.
III) Comparing and weighing of structural properties	Looking at the branching of the nucleophiles as well as the bond length of C-O and C-S and the resulting electronic repulsion, the steric hindrance in the case of the sulfur nucleophile is not to be classified as significantly greater than that of the oxygen nucleophile. However, the sulfur nucleophiles' branched backbone and its electronic structure results in an increased repulsive interaction with the electrophile, which leads to a slightly more difficult approaching of the sulfur nucleophile to the electrophilic center in this interaction than in the upper reaction. However, the increased polarizability of the sulfur nucleophile compared to the oxygen nucleophile, as well as the increased electron donation via inductive effects of the increased number alkyl groups, supports the nucleophilic attack; i.e., the bond formation between the nucleophile and the electrophile is facilitated, which outweighs the effect of the repulsive interactions.
IV) Making a claim based upon structural properties	Based on the structural considerations, the sulfur nucleophile can be considered the better nucleophile.
V) Linking structural claim to energetics	Compared to the transition state in reaction A, the transition state in reaction B is energetically lowered due to the supportive structural influencing factors.
Final decision	That's why reaction B occurs faster.

9.2. Supporting Information 2: Excerpt of the Semi-structured Interview-protocol

Table S2. Excerpt of the semi-structured interview-protocol.

Situation	**Prompt**
Beginning	If you were to compare the reactions, which of the two reactions occurs faster. Take your time, and look at it first; then, **explain** your decision in detail. Again, the task and questions are designed to help us understand you better, not to test your performance. Questions are asked to help understand your thought processes and, in general, the thought processes of students.
Situation	**Excerpt of potential prompts (only used if a participant attempted to elaborate in this direction)**
Regarding the explicit differences	How do the reactions differ? Where do you see XY?
Regarding implicit properties	From what part of the structural formula did you derive that? What makes you think this is relevant to this response? Why does this seem important to you here? How would you define (property XY)?
Regarding the influence on the reaction process	What influence/effect does that have (that there are more alkyl groups on it/that there is a sulfur atom)?
Regarding comparing and weighing	If I understand you correctly, you had (XY) arguments. In which directions do your arguments point?
Regarding the claim	Which reaction do you choose, and what are you basing your decision on?
Regarding connecting structural and energetic considerations/ energetic claim	What does “stable” mean to you? How does this influence the energetic course of the reactions? Can you tell me a bit more about the activation energy of the reactions? How do you come to such a conclusion?
Exploring the approach	How do you solve such a task? Which steps do you follow to come to a task solution? Could you explain to a fellow student or to me how to approach the task?
Pause	What is irritating you? Why are you struggling?Tell me what you are thinking about now. I know you have explained this to me before. However, please help me to understand you better by explaining it to me again.
Inaccurate wording/ phrases/slang/humanization: e.g., "better“, “easier“, “wants to“	Can you please explain in more detail? What is meant by "[XY]"?
Incorrect statement	Avoid suggestions! Ask, e.g., what do you mean by that?
Perplexity/uncertainty	What would help you answer the question?
In the end	Did you forget anything else? Is there anything else you would like to add?
Additionally in the post-interview:	
Regarding the approach	Did anything change in your approach compared to the last interview? How did [XY] change?, What was easy/easier//hard/harder for you?
Evaluating the videos	If you recall the videos, can you remember a general approach (to solving case comparison tasks)? How did you like the highlighting? Do you think the highlights were helpful for learning? How did you feel about the verbal explanation and the visualization? (…)

9.3. Supporting Information 3: Coding System

Table S3. Coding system to identify reasoning steps in the students' explanations.

Reasoning step	Code	Description	Examples
RQ1:			
I) Infer structural properties	Electronegativity	Participant infers structural property of electronegativity of the heteroatoms and/or describes the tendency to attract bonding electrons.	"Oxygen is more electronegative compared to sulfur…" "Oxygen attracts the electrons of the bond more to itself"
	Polarizability	Participant infers the structural property of polarizability of the heteroatoms and/or describes electron shielding with electron movement (of an electron cloud) toward the electrophilic center.	"Sulfur is more polarizable…" "Sulfur has more loosely held electrons because of the shielding effect of the nucleus…they are more attracted to the electrophilic carbon compared to oxygen"
	Inductive effects	Participant infers the structural property of inductive effects regarding the backbone of the nucleophile and/or describes electron-donation of the alkyl groups (electron-pushing/withdrawing along bonds)	"The surrounding C atoms stabilize the charge due to inductive effects" "The alkyl group has inductive effects that can push electrons"
	Steric hindrance	Participant infers the structural property of steric hindrance of the backbone of the nucleophile and/or describes that electronic repulsions (of orbitals) may occur	"The additional CH group interferes with the nucleophilic attack because it becomes tight, so it's sterically hindered." "The alkyl group leads to hindrance as the electrons repel each other".
II) Verbalize the influence on the reaction process		Participant verbalizes how a structural property affects the course of the reaction.	"Oxygen is more electronegative, so electrons are less willingly provided for bond formation." "Sulfur is slightly more polarizable, it's electrons are better available for bond formation." "Due to decreased steric hindrance, the nucleophilic attack is better here."
RQ2:			
Reasoning step	**Code**	**Description**	**Examples**
III) Compare and weigh structural properties		Participant compares/weighs structural properties and refers to several concepts in their explanation.	"On the one hand, we have inductive effects of the alkyl groups pushing electrons. On the other hand, there is steric hindrance...their influences have to be balanced." "The size and the more polarizable sulfur speaks for reaction B, electronegativity of the oxygen atom for A…"
IV) Make a claim based on a structural property/several properties		Participant uses a structural property/uses several properties to make a claim.	"I choose reaction A because oxygen is more electronegative." "Due to the alkyl groups' electron donation to the sulfur in reaction B and it's higher polarizability, I think reaction B is the faster one"
V) Link structural claim to energetics		Participant refers to energy and thus establishes a link between structural considerations and energetic course of the reaction.	(not provided by students) …hence, B has a lower activation energy and proceeds faster. ...based on the structural considerations, for example the influence of polarizability and inductive effects, the sulfur nucleophile can be considered the better nucleophile. Compared to the transition state in reaction A, the transition state in reaction B is energetically lowered due to the supportive structural influencing factors. Therefore, reaction B occurs faster.

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10. Appendix

10.1. First Study: Consent Form

Einwilligungserklärung zur Erhebung und Verarbeitung personenbezogener Daten für Forschungszwecke

Gegenstand des Forschungsprojektes

1.	Forschungsprojekt	EYE-OC
2.	Forschungszweck	Entwicklung und Evaluation eines innovativen Instruktionsansatzes zur Verbesserung des Verständnisses von Reaktionsmechanismen bei Chemie-Studierenden im Rahmen der Einführungsveranstaltung zur Organischen Chemie
3.	Durchführende Institutionen	Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN), Didaktik der Chemie, Olshausenstr. 62, 24118 Kiel Justus-Liebig-Universität Gießen, Institut für Didaktik der Chemie, Heinrich-Buff Ring 17, 35392 Gießen
4.	Projektleitung	Dr. Sascha Bernholt (IPN Kiel, Tel.: 0431-8803160, Email: bernholt@ipn.uni-kiel.de) Prof. Dr. Nicole Graulich (JLU Gießen, Tel.: 0641-9934600, Email: nicole.graulich@didaktik.chemie.uni-giessen.de)
5.	Erhebungszeitraum	Juni /Juli 2018
6.	Interviewerin/Interviewer	Julia Eckhard, Marc Rodemer

Einwilligungserklärung

Hiermit willige ich ein, dass im Rahmen des unter (1) beschriebenen Forschungsprojekts Daten meiner Person erhoben und ausgewertet werden. Die Erhebung erfolgt zum einen durch **Audioaufnahmen**, die in der Folge transkribiert werden. Zum anderen werden **Blickbewegungsaufnahmen** erhoben.

Daten aus beiden Erhebungsformaten werden vollständig pseudonymisiert (s.u.) und für wissenschaftliche Analysen und in der Folge für wissenschaftliche Veröffentlichungen verwendet und mindestens 10 Jahre lang gespeichert werden.

Ich bin damit einverstanden, dass

□ Ja □ Nein	pseudonymisierte **Transkriptausschnitte, Audioausschnitte** und **Blickbewegungsaufnahmen** auszugsweise Gegenstand von *wissenschaftlichen Arbeiten und Publikationen* sind.
□ Ja □ Nein	pseudonymisierte **Transkriptausschnitte**, **Audioausschnitte** und **Blickbewegungsaufnahmen** zu *Lehrzwecken* verwendet werden.

Sofern ich besondere Kategorien von personenbezogenen Daten angebe bzw. angegeben habe, sind diese von der Einwilligungserklärung umfasst.

Pseudonymisierung

Die Aufzeichnung und Auswertung der Daten erfolgt im IPN Kiel bzw. der JLU Gießen (vgl. 1.3) unter Verwendung eines persönlichen Codewortes, das ich selbst erstellt habe. Das Codewort ist so aufgebaut, dass niemand von meinem Codewort auf meine Person rückschließen kann, auch das Projektteam nicht. Ich selbst kann mein Codewort aber jederzeit rekonstruieren, wenn ich danach gefragt werde und es vergessen haben sollte.

Dies sind die Bestandteile des Codeworts:

- Die beiden letzten Buchstaben des Geburtsnamens Ihrer Mutter
- Die Anzahl der Buchstaben des (ersten) Vornamens Ihrer Mutter
- Die beiden letzten Buchstaben des (ersten) Vornamens Ihres Vaters
- Ihr eigener Geburtstag (nur der Tag, nicht Monat und/oder Jahr).

Über Art und Umfang von Erhebung und Auswertung wurde ich mündlich und in der schriftlichen Anlage zu dieser Erklärung umfassend informiert. Sofern ich Fragen zu dieser vorgesehenen Studie hatte, wurden sie mir vollständig und zu meiner Zufriedenheit beantwortet.

Die Mitglieder der beteiligten Arbeitsgruppen sind zur Verschwiegenheit gegenüber Dritten verpflichtet. Gleichermaßen erkläre ich Verschwiegenheit bezüglich der Aufgabeninhalte gegenüber Dritten.

Ich wurde auch darüber informiert, dass während der Aufzeichnung mit dem Eye-Tracker photosensitive Epilepsie auftreten könnte.

Ihre Einwilligung ist freiwillig. Sie können die Einwilligung ablehnen, ohne dass Ihnen dadurch irgendwelche Nachteile entstehen. Ihre Einwilligung können Sie jederzeit gegenüber der durchführenden Institution widerrufen. Die weitere Verarbeitung Ihrer personenbezogenen Daten wird ab diesem Widerruf unzulässig. Dies berührt jedoch nicht die Rechtmäßigkeit der aufgrund der Einwilligung bis zum Widerruf erfolgten Verarbeitung. Relevante Definitionen der verwendeten datenschutzrechtlichen Begriffe sind in der Anlage Begriffsbestimmungen enthalten.

_____	_____	_____
Vorname und Nachname in Druckschrift	Datum	Unterschrift

Informationen über die Erhebung und Verarbeitung Ihrer personenbezogenen Daten

Kurzdarstellung der am Forschungsprojekt Beteiligten

Das Forschungsprojekt wird durchgeführt von Dr. Sascha Bernholt (Projektleitung; Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN), Didaktik der Chemie, Olshausenstr. 62, 24118 Kiel) und Prof. Dr. Nicole Graulich (Projektleitung; Justus-Liebig Universität Gießen, Institut für Didaktik der Chemie, Heinrich-Buff Ring 17, 35392 Gießen), Prof. Dr. Melissa Weinrich (Kooperationspartnerin; University of Northern Colorado, Department of Chemistry and Biochemistry, Greeley, CO 80639), Julia Eckhard (Wiss. Mitarbeiterin, Justus-Liebig Universität Gießen) und Marc Rodemer (Wiss. Mitarbeiter; IPN Kiel). Das Projekt wird gefördert von der Deutschen Forschungsgemeinschaft (DFG; BE4703/5-1 bzw. GR4003-3-1).

Alle Beteiligten, die Zugang zu den Daten erhalten sind auf das Datengeheimnis verpflichtet.

Zweck der Datenverarbeitung

Die Erhebung und Verarbeitung der Daten dient alleine für die in 1.2. genannten wissenschaftlichen Zwecke.

Ihre Kontaktdaten werden gesondert und ausschließlich für die Projektleitung zugänglich gespeichert. Dies dient der Dokumentation ihrer Einverständniserklärung und einer möglichen Identifizierung Ihrer Daten falls Sie diese Einwilligung später widerrufen.

Art der Datenverarbeitung

Die Gespräche während der Erhebung werden aufgezeichnet, die Aufnahmen abgetippt und pseudonymisiert. Auch die Blickbewegungsaufnahmen werden pseudonymisiert. Bei der Pseudonymisierung werden Personennamen, Ortsnamen und Berufsbezeichnungen, Kontaktdaten wie E-Mailadressen oder Telefonnummern ersetzt. Ihr Name und Ihre Kontaktdaten werden für die datenschutzrechtliche Dokumentation gesondert gespeichert. Zugriff hierauf hat ausschließlich die Projektleitung (s. 1.4).

In Veröffentlichungen oder zu Lehrzwecken können auszugsweise pseudonymisierte Zitate oder Aufnahmen wiedergegeben werden, wenn Sie dem explizit unter (2) zugestimmt haben.

Eine Verarbeitung Ihrer personenbezogenen Daten zum Zweck einer automatisierten Entscheidungsfindung (einschließlich Profiling) gemäß Art. 22 Abs. 1 und Abs. 4 DSGVO findet nicht statt.

Kategorien der zu verarbeitenden Daten

Offene Interviews können naturgemäß alle möglichen Arten von Daten enthalten. Insb. können hierbei besondere Kategorien enthalten sein, die Aufschluss geben über rassische und ethnische Herkunft, politische Meinungen, religiöse oder weltanschauliche Überzeugungen, Gewerkschaftszugehörigkeit, Gesundheitsdaten oder Daten zum Sexualleben oder der sexuellen Orientierung einer natürlichen Person, auch wenn keine dieser Kategorien Ziel dieser Erhebung ist.

Kontaktdaten der datenverarbeitenden Stelle

Bei Fragen, Auskunftswünschen oder dem Widerruf Ihrer Einwilligung wenden Sie sich bitte an:

Projektleitung		Datenschutzbeauftragter
Dr. Sascha Bernholt Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN) Didaktik der Chemie Olshausenstr. 62 24118 Kiel Tel.: 0431-8803160 Email: bernholt@ipn.uni-kiel.de	Prof. Dr. Nicole Graulich Justus-Liebig Universität Gießen Institut für Didaktik der Chemie Heinrich-Buff Ring 17 35392 Gießen Tel.: 0641-9934600 Email: nicole.graulich@didaktik.chemie.uni-giessen.de	Prof. Dr. Olaf Köller Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN) Erziehungswissenschaft Olshausenstr. 62 24118 Kiel Tel.: 0431-8803120 Email: koeller@ipn.uni-kiel.de

Rechtsgrundlage

Wir verarbeiten die von Ihnen erhobenen personenbezogene Daten auf Basis Ihrer Einwilligung gemäß § 4 Abs. 1 Bundesdatenschutzgesetz (BDSG) und mit Geltung der Datenschutzgrundverordnung (DSGVO), ab dem 25. Mai 2018, gemäß Art. 6 Abs. 1 lit. a DSGVO. Sofern besondere Kategorien personenbezogener Daten betroffen sind, verarbeiten wir die von Ihnen erhobenen personenbezogenen Daten auf Basis Ihrer Einwilligung gemäß § 4 Abs. 1 BDSG und mit Geltung der Datenschutzgrundverordnung (DSGVO) gemäß Art. 9 Abs. 2 lit. a DSGVO.

Empfänger oder Kategorien von Empfängern

Ihre Daten werden ausschließlich von den unter 3.1 genannten Institutionen genutzt.

Dauer der Speicherung / Kriterien für die Festlegung der Dauer

Ihre personenbezogenen Daten werden gespeichert, solange Sie Ihre Einwilligung nicht widerrufen haben und eine Notwendigkeit zur Erreichung des unter 1.2. genannten Zwecks der Verarbeitung, mindestens 10 Jahre, oder eine Pflicht zur Aufbewahrung bestehen. Andernfalls werden Ihre personenbezogenen Daten nach Maßgabe der Anforderungen des Datenschutzrechts gelöscht.

Ihre Rechte

Im Rahmen der gesetzlichen Vorgaben haben Sie gegenüber uns grundsätzlich Anspruch auf:

- Bestätigung, ob Sie betreffende personenbezogenen Daten verarbeitet werden,
- Auskunft über diese Daten und die Umstände der Verarbeitung,
- Berichtigung, soweit diese Daten unrichtig sind,
- Löschung, soweit für die Verarbeitung keine Rechtfertigung und keine Pflicht zur Aufbewahrung (mehr) besteht,
- Einschränkung der Verarbeitung in besonderen gesetzlich bestimmten Fällen und
- Übermittlung Ihrer personenbezogenen Daten – soweit Sie diese bereitgestellt haben – an Sie oder einen Dritten in einem strukturierten, gängigen und maschinenlesbaren Format.

Darüber hinaus haben Sie das Recht, Ihre Einwilligung jederzeit zu widerrufen, mit der Folge, dass die Verarbeitung Ihrer personenbezogenen Daten, nach Maßgabe Ihrer Widerrufserklärung, durch diesen oder durch beide Projektpartner für die Zukunft

unzulässig wird. Dies berührt die Rechtmäßigkeit der aufgrund der Einwilligung bis zum Widerruf erfolgten Verarbeitung jedoch nicht.

Schließlich möchten wir Sie auf Ihr Beschwerderecht bei der Aufsichtsbehörde hinweisen.

Photosensitive Epilepsie

Manche Menschen mit photosensitiver Epilepsie sind anfällig für epileptische Anfälle oder Bewusstseinsverlust, wenn sie bestimmten Blitzlichtern oder Lichtmustern im täglichen Leben ausgesetzt sind. Dies kann auch passieren, wenn die Person keine Epilepsie-Anamnese hat oder nie epileptische Anfälle hatte. Eine Person mit photosensitiver Epilepsie würde wahrscheinlich auch Probleme mit Fernsehbildschirmen, einigen Computerspielekonsolen und flackernden Leuchtstofflampen haben. Solche Personen können einen Anfall haben, während sie bestimmte Bilder oder Muster auf einem Monitor sehen oder sogar wenn sie den Lichtquellen eines Eye-Trackers ausgesetzt sind. Es wird geschätzt, dass etwa 3-5% der Menschen mit Epilepsie diese Art von photosensitiver Epilepsie haben. Viele Menschen mit photosensitiver Epilepsie erleben eine "Aura" oder fühlen sich seltsam, bevor der Anfall auftritt. Wenn Sie sich während der Erhebung merkwürdig fühlen, weisen Sie uns darauf hin und drehen sich vom Eye-Tracker weg.

Anlage: Begriffsbestimmungen

- „Personenbezogene Daten“ sind gemäß Art. 4 Nr. 1 DSGVO alle Informationen, die sich auf eine identifizierte oder identifizierbare natürliche Person (im Folgenden „betroffene Person“) beziehen. Als identifizierbar wird eine natürliche Person angesehen, die direkt oder indirekt, insbesondere mittels Zuordnung zu einer Kennung wie einem Namen, zu einer Kennnummer, zu Standortdaten, zu einer Online-Kennung oder zu einem oder mehreren besonderen Merkmalen identifiziert werden kann, die Ausdruck der physischen, physiologischen, genetischen, psychischen, wirtschaftlichen, kulturellen oder sozialen Identität dieser natürlichen Person sind. Das kann z.B. die Angabe sein, wo eine Person versichert ist, wohnt oder wie viel Geld er oder sie verdient. Auf die Nennung des Namens kommt es dabei nicht an. Es genügt, dass man herausfinden kann, um welche Person es sich handelt.

- „Besondere Kategorien“ personenbezogener Daten sind gemäß Art. 9 Abs. 1 DSGVO Daten, aus denen die rassische und ethnische Herkunft, politische Meinungen, religiöse oder weltanschauliche Überzeugungen oder die Gewerkschaftszugehörigkeit hervorgehen, sowie die Verarbeitung von genetischen Daten, biometrischen Daten zur eindeutigen Identifizierung einer natürlichen Person, Gesundheitsdaten oder Daten zum Sexualleben oder der sexuellen Orientierung einer natürlichen Person.

- „Gesundheitsdaten“ sind gemäß Art. 4 Nr. 15 DSGVO personenbezogene Daten, die sich auf die körperliche oder geistige Gesundheit einer natürlichen Person, einschließlich der Erbringung von Gesundheitsdienstleistungen, beziehen und aus denen Informationen über deren Gesundheitszustand hervorgehen.

- „Verarbeitung“ ist gemäß Art. 4 Nr. 2 DSGVO jeder mit oder ohne Hilfe automatisierter Verfahren ausgeführten Vorgang oder jede solche Vorgangsreihe im Zusammenhang mit personenbezogenen Daten wie das Erheben, das Erfassen, die Organisation, das Ordnen, die Speicherung, die Anpassung oder Veränderung, das Auslesen, das Abfragen, die Verwendung, die Offenlegung durch Übermittlung, Verbreitung oder eine andere Form der Bereitstellung, den Abgleich oder die Verknüpfung, die Einschränkung, das Löschen oder die Vernichtung.

10.2. First Study: Guidelines for the Qualitative Interview & Interview Protocol

Interviewleitfaden

1. Begrüßung

- Formalia
  - Grund der Studie: Wir wollen die Erklärungen und Blickmuster von Studierenden beim Umgang mit organischen Reaktionen analysieren.
- Einverständniserklärung unterschreiben lassen, dass Messungen und Messdaten für Forschungszwecke verwendet werden dürfen und ggf. in der Lehre eingesetzt werden dürfen.
- Demografische Angaben
  - Alter, Geschlecht, Studienfächer, Semesterzahl, OC besucht j/n, OC bestanden j/n, In der Lehre seit x Jahren,

Vorbereitung zum Eye-Tracking:

- Handy aus?
- Brille notwendig?

- Erwartungen:
  - Es gibt 8 Aufgaben. Pro Aufgabe sind zwei Reaktionen zu sehen, die sich minimal unterscheiden. Jede Reaktion ist vollständig abgebildet, das heißt mit Edukten, Produkten und Elektronenpfeilen. Es wird jeweils gefragt, welche der zwei Reaktionen A oder B schneller abläuft.
  - Alle Reaktionen stammen aus dem Bereich „Nukleophile Substitution“
  - Es gibt 2 Blöcke. Im ersten Block sollen Sie die Aufgaben für sich selbst lösen und im zweiten Block einem Studierenden erklären. Zwischen beiden Blöcken gibt es eine kurze Pause zum kalibrieren des Eye-Trackers.

- Jede Aufgabe wird 2 mal bearbeitet. Die Aufgaben sollen zuerst still angesehen und danach erklärt werden. Bitte geben Sie Bescheid, wenn Sie zur nächsten Phase gehen wollen.
- Nach jeder Phase soll zur nächsten Folie geklickt werden.
- In der ersten Phase beim “Still betrachten” sollen Sie die Reaktionen ansehen und vergleichen. Entscheiden Sie, welche Reaktion schneller abläuft.
- In der zweiten Phase beim “Laut denken” teilen Sie mir Ihre Entscheidung mit, welche der Reaktionen schneller verläuft. Das heißt Lösung sagen, Reaktionen und Unterschiede beschreiben und eine Begründung für die Entscheidung liefern.
- Es folgt eine kurze Pause, danach wird der Eye-Tracker kalibriert.
- Im zweiten Block sollen Sie die Aufgaben einem Studierenden mit geringem Vorwissen erklären.

- Zwischenfragen
  - In Phase 2 dem „Laut Denken“ stelle ich Ihnen Zwischenfragen. Meistens soll ein Teil der Aufgabe genauer beschrieben werden oder ein Bezug erklärt werden. Manchmal wird auch konkret inhaltlich gefragt.

- Verhalten beim Eye Tracking
  - Während des Eye Trackings bitte still sitzen bleiben. Nicht zu sehr bewegen, d.h. Stuhl und Sitzposition vorher einstellen. Sitzen Sie aufrecht. Auch wenn der Interviewer spricht, soll der Kopf nicht gedreht werden, das verschlechtert die Kalibrierung. Sprechen Sie deutlich. Nicht die Hände/Haare zwischen Augen und den Eye-Tracker führen.
  - Leiden Sie an photosensitiver Epilepsie? Ja/nein?

2. Testung / Beginn des Eye Trackings!

1. Kalibrierung
2. Beispielablauf der Phasen mit Beispielaufgabe
3. Aufgaben
   3.1. Ansehen: richtige Lösung suchen, nicht reden
   3.2. Laut Denken: Lösung sagen, Aufgabe und Unterschiede beschreiben und begründend erklären

Interviewprotokoll

Situation	Reaktion
• Ungenaue Formulierung • Austauschbare Phrasen: ○ „energetisch günstiger“ ○ „stabiler“	Was meinen Sie damit? Können Sie mir das genauer erklären? Was ist mit „[stabiler]“ gemeint?
Falsche Äußerungen	Achtung: Nicht beeinflussen, keine Suggestion, nur nachfragen, z.B. Was meinen Sie damit?
Nennung einer impliziten Eigenschaft	Von welchem Teil der Struktur haben Sie das abgeleitet? Wie kommen Sie darauf, dass das für diese Reaktion relevant ist? Warum erscheint Ihnen das hier wichtig? Woran machen Sie das fest?
Pause	Sagen Sie mal, woran Sie jetzt denken. [Meta Ebene anbieten] Ich weiß, Sie haben das jetzt schon einmal erläutert. Aber Sie helfen mir, das besser zu verstehen, wenn Sie das jetzt noch einmal beschreibe.
Umgangssprache, Vermenschlichung „Leichter“, „Umklappen“, „besser“	Fragen, ob die gerade gesagte Aussage generalisierbar ist. Erinnern Sie sich an andere Reaktionen, bei denen das wichtig ist?
Schluss	Bevor weiter geklickt wird: Für welche Reaktion haben Sie sich entschieden? Haben Sie noch etwas vergessen? Möchten Sie noch etwas ergänzen? Wenn nicht, gehen Sie bitte zur nächsten Aufgabe.

3.3. Jmd. Erklären: Hier ist die Lösung vorgegeben. Bitte erklären Sie die Reaktionen einem Studierenden mit geringem Vorwissen.

3.4. Ende des Eye Trackings

Nach dem Interview

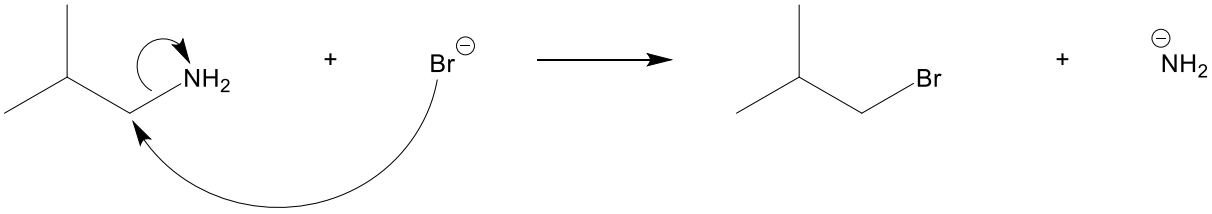
- Haben Sie eigene Ergänzungen oder Kommentare?
- Ist Ihnen noch etwas aufgefallen?
- Evaluation der Contrasting Cases
  - Fanden Sie diesen Aufgabentyp mit den Vergleichen hilfreich/ verwirrend
- Strategie der Herangehensweise (bekannte Aufgabe zeigen)
  - Wie sind Sie allgemein vorgegangen?

10.3. First Study: Sample Solutions for the Interview Tasks

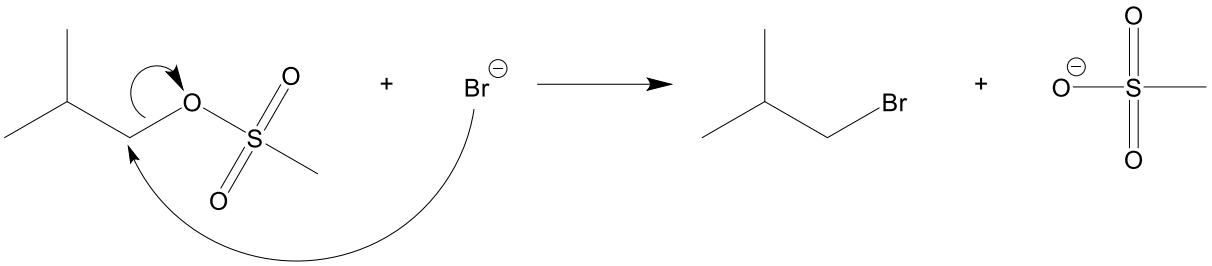
Aufgabenlösungen (nur für Interviewer):

Aufgabe 2:

A



B



Aufgabe	Aufgabentyp	Konzepte	„false friends“	Ziele
BB	Abgangsgruppe	Mesomeriestabilsierung Basizität (Nukleophilie)		Diskussion us. AG→ Stabilität von Basen strukturelle / energetische Aspekte diskutieren

Erklärung:

In den folgenden Fällen reagieren A Isobutylamin und B Isobutylmesylat je in einer S_N2-Reaktion zu Isobutylbromid (1-Brom-2-methylpropan).

Die S_N2-Reaktion läuft in der Richtung ab, in der es der stärkeren Base erlaubt ist, die schwächere zu verdrängen. Je stärker eine Base, desto bereitwilliger teilt eine Verbindung ihre freien Elektronenpaare mit anderen Verbindungen (wie stark die Tendenz ist ein Proton aufzunehmen).

Im CC ist die Abgangsgruppenneigung zu vergleichen und die schwächere Base zu identifizieren. Die Qualität der Abgangsgruppe ist allgemein abhängig von der Stärke der C-Abgangsgruppen-Bindung und der Stabilität der Abgangsgruppe.

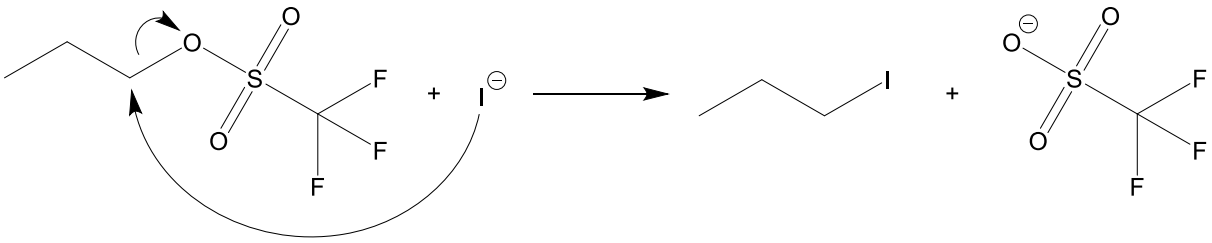
Je geringer die Basizität einer Gruppe, desto besser ihre Abgangsgruppeneigenschaften, da schwächere Basen stabilere Basen sind. Von guten Abgangsgruppen (= schwachen Basen) werden bereitwillig Elektronen getragen, die sie zuvor mit einem Bindungspartner teilten. Weiterhin sind schwache Basen nicht so stark gebunden wie starke Basen. In diesem Fall ist das Mesylat (Methylsulfonat) die bessere Abgangsgruppe im Vergleich zur Amingruppe, da die negative Ladung über drei mesomere Grenzstrukturen verteilt ist. Je

größer die Zahl relativ stabiler mesomerer Grenzformeln, desto größer die Stabilisierung (desto höher die Resonanzenergie). Die Amin-Gruppe weist eine lokalisierte negative Ladung auf und ist eine sehr starke Base. Als Abgangsgruppe ist das Amin-Ion ein Hochenergieteilchen und deswegen läuft Reaktion B bevorzugt ab.

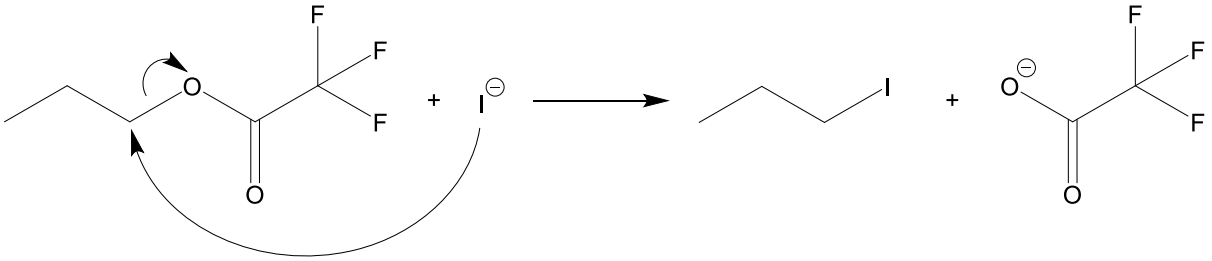
Energetische Betrachtung:
ÜZ der Reaktion B liegt im Vergleich zu A niedriger, dadurch, dass die C-Mesylat-Bindung schwächer ist und aufgrund der Mesomeriestabilisierung des Mesylat-Ions (=schwache Base).

Aufgabe 3:

A



B



Erklärung:

Aufgabe	Aufgabentyp	Konzepte	„false friends“	Ziele
	Abgangsgruppe	Mesomeriestabilisierung Basizität (Nukleophilie)	-CF_3 nicht als elektronenzeihende Gruppe erkennbar	Diskussion us. AG→ Stabilität von Basen strukturelle / energetische Aspekte diskutieren

Im Folgenden reagieren A Propyltriflat und B Propyltrifluoracetat je in einer S_N2-Reaktionen zu 1-Iodpropan. Es handelt sich um S_N2-Reaktionen, bei denen Iodid als gutes Nukleophil zwei gute Abgangsgruppen substituiert.

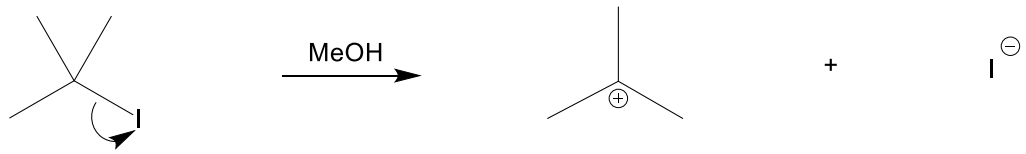
Die S_N2-Reaktion läuft in der Richtung ab, in der es der stärkeren Base erlaubt ist, die schwächere zu verdrängen. Je stärker eine Base, desto bereitwilliger teilt eine Verbindung ihre freien Elektronenpaare mit anderen Verbindungen (wie stark die Tendenz ist ein Proton aufzunehmen).
Im CC ist die Abgangsgruppenneigung zu vergleichen und die schwächere Base zu identifizieren. Die Qualität der Abgangsgruppe ist allgemein abhängig von der Stärke der C-Abgangsgruppen-Bindung und der Stabilität der Abgangsgruppe.
Je geringer die Basizität einer Gruppe, desto besser ihre Abgangsgruppeneigenschaften, da schwächere Basen stabilere Basen sind. Von guten Abgangsgruppen (= schwachen Basen) werden bereitwillig Elektronen getragen, die sie zuvor mit einem Bindungspartner teilten. Weiterhin sind schwache Basen nicht so stark gebunden wie starke Basen. In diesem Fall ist das Triflat die bessere Abgangsgruppe im Vergleich zur Trifluoracetat-Gruppe, da die negative Ladung über drei anstatt zwei mesomere Grenzstrukturen verteilt ist. Je größer die Zahl relativ stabiler mesomerer Grenzformeln, desto größer die Stabilisierung (desto höher die Resonanzenergie) – die Anzahl der mesomeren Grenzstrukturen ist im Falle des Triflats größer. Reaktion A läuft bevorzugt ab.

Weiterhin kann über die Säurestärke argumentiert werden. Trifluormethylsulfonsäure, die korrespondierende Säure zum Triflat-Ion, ist die stärkere Säure im Vergleich zur Trifluoressigsäure.

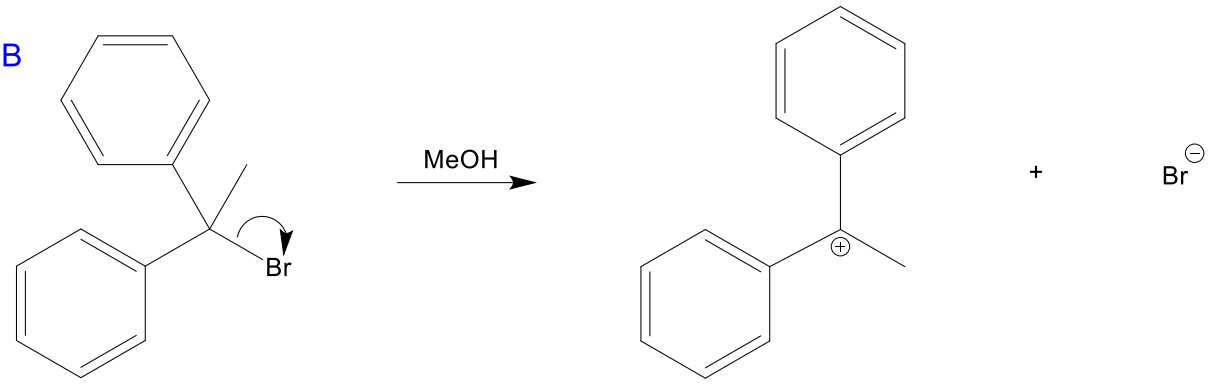
Energetische Betrachtung:
ÜZ der Reaktion B liegt im Vergleich zu A niedriger, dadurch, dass die C-Triflat-Bindung schwächer ist und aufgrund der Mesomeriestabilisierung des Triflat-Ions (=schwache Base).

Aufgabe 4:

A



B



Erklärung:

Aufgabe	Aufgabentyp	Konzepte	„false friends“	Ziele
	Abgangsgruppe Substrateffekt	Mesomerie Hyperkonjugation Basizität	Abwägung ➔ Zwei Effekte, die zu Verwirrung führen könnten	Diskussion über Abgangsgruppenqualität, Stabilität von ÜZ/Carbenium-Ionen strukturelle / energetische Aspekte diskutieren

Bei den beiden Reaktionen A und B wird die Bildung von jeweils einem tertiären Carbenium-Ion gezeigt, es handelt sich um eine Solvolyse-Reaktion.
Im CC ist zum einen die Abgangsgruppenneigung zu vergleichen und die schwächere Base zu identifizieren und zum anderen die Substrate/bzw. Carbenium-Ion-Stabilitäten zu vergleichen, also zwei Merkmale zu unterscheiden. Bei Reaktion A ist die Abgangsgruppe ein Iodid-Ion, bei Reaktion B ein Bromid-Ion. Bei A sind die Substrate drei Methylgruppen, bei B sind es zwei Phenylgruppen und eine Methylgruppe.

Je geringer die Basizität einer Gruppe, desto besser ihre Abgangsgruppeneigenschaften, da schwächere Basen stabilere Basen sind. Von guten Abgangsgruppen (= schwachen Basen) werden bereitwillig Elektronen getragen, die sie zuvor mit einem Bindungspartner teilten. Weiterhin sind schwache Basen nicht so stark gebunden wie starke Basen. Iodid ist in einem protischen LM die bessere Abgangsgruppe (geringere Basizität), da es im Vergleich zum Bromid aufgrund der größeren Atomgröße diffusere Elektronen aufweist und „polarisierbarer“ ist. Die Elektronen werden im Vergleich zum Bromid bereitwilliger „getragen“.

Durch die Phenylreste bei Reaktion B findet eine Mesomeriestabilisierung des Carbenium-Ions statt, welche bei den Methylresten nicht stattfindet (hier nur +I-Effekt/neunfache Hyperkonjugation). Im Fall A verläuft die Stabilisierung des tertiären Carbenium-Ions über Hyperkonjugation (+*I*-Effekt; Elektronendichte einer benachbarten *σ*-Bindung wird in das leere p-Orbital doniert) durch die Methylgruppen (neunfache Hyperkonjugation). Das Carbenium-Ion bei Reaktion B ist also aufgrund der Elektronendelokalisation über π-Bindungen (mesomerer Elektronenschub) stabiler. Es ließen sich noch weitere sechs Grenzformeln schreiben.
Weiterhin sind Lösungsmittel-Effekte zu beachten. In beiden Fällen erfolgt die Solvatation der Ionen Iodid und Bromid über Wasserstoffbrückenbindungen. Die Stärke der sich ausbildenden Wasserstoffbrückenbindungen, die zudem zu einem Energiegewinn führt, sollte beim Bromid etwas stärker sein.

Energetische Betrachtung:
Der geschwindigkeitsbestimmende Schritt der S_N1-Reaktion entspricht der Bildung der carbokationischen Zwischenstufe (HAMMOND-Postulat). Die Energie des zugehörigen ÜZ, bestimmt die Gesamtgeschwindigkeit der Reaktion und steht in Abhängigkeit zur Stabilität des Carbenium-Ions. Im Vergleich lässt sich sagen, dass die Aktivierungsenergie zur Eliminierung der Abgangsgruppe im Fall A mit Iodid zwar geringer ist; der ÜZ/das Carbenium-Ion durch den +*M*-Effekt der Phenylreste sowie des +*I*-Effekts der Methyl-Gruppe im Fall B jedoch besser stabilisiert werden kann. Reaktion B läuft schneller ab als Reaktion A.

Quellen:

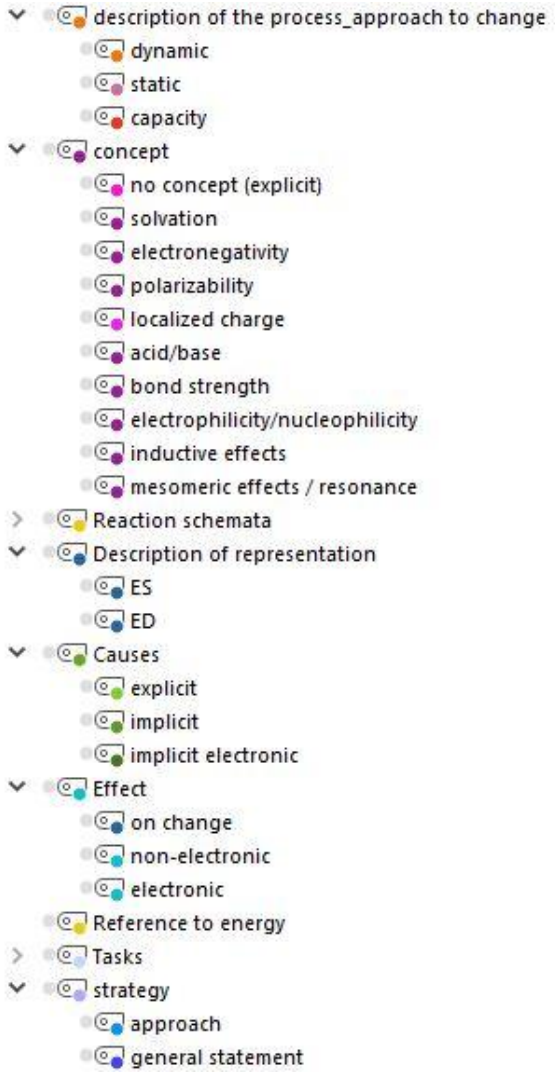
Bruice, P. Y. (2011). *Organische Chemie: studieren kompakt*. Pearson Deutschland GmbH.

Clayden, J., Greeves, N., & Warren, S. (2012). Organic Chemistry. Oxford University Press, USA.

Schmitt, C.; Schween, M. Konzepte verstehen anhand vergleichender qualitativer Kinetik-Messungen bei S_N1-Reaktionen: Die Wirkung von Mesomerie und Hyperkonjugation im Vergleich. CHEMKON 2021, 28 (2), 74-81.

Vollhardt, K. P. C., & Schore, N. E. (2011). *Organische Chemie*. John Wiley & Sons.

10.4. Coding System Used in the First Study



10.5. Second Study: Consent Form and Demographic Questionnaire

Information zum wissenschaftlichen Untersuchungsvorhaben EYE OC

Liebe Teilnehmerinnen und Teilnehmer,
unser Projekt befasst sich mit der Entwicklung und Evaluation von Lernmaterialien zur Verbesserung des Verständnisses von Reaktionsmechanismen bei Chemiestudierenden. Dazu ist eine wissenschaftliche Untersuchung geplant, die zu drei hintereinander stattfindenden Zeitpunkten insgesamt **zwei Interviews und zwei Fragebögen** umfasst.
Im Rahmen dessen werden auch personenbezogene Daten erhoben. Hierbei handelt es sich um folgende: Studiengang, Semester und Abiturnote. Außerdem werden im Rahmen der Interviews Tonaufnahmen sowie Filmaufnahmen des Tisch-/Handbereichs gemacht.
Um die einzelnen Messzeitpunkte und Erhebungsinstrumente bzw. Interviews einander zuordnen zu können, wird zu den einzelnen Messzeitpunkten ein Code erfragt, den Sie selbst generieren. Es werden keine Listen mit Namen und zugehörigen Codes angelegt.
Die Teilnahme an der Untersuchung ist freiwillig und unter Angabe des Codes widerrufbar. Aus einer Nichtteilnahme erwachsen Ihnen keine Nachteile. Alle erhobenen Daten werden streng vertraulich behandelt und nur zu wissenschaftlichen Zwecken genutzt. Die Daten werden nicht an Dritte weitergegeben. Eine Zuordnung der erhobenen Daten zu einzelnen Personen ist nicht möglich. Sollten während der Interviews unaufgefordert persönliche Informationen preisgegeben werden, die Rückschlüsse auf Ihre Person zulassen würden, so werden diese Teile gelöscht und nicht dauerhaft gespeichert.
Um die Teilnahme an unserer Studie zu ermöglichen, bitten wir darum, die beiliegende Einverständniserklärung zu unterzeichnen. Die Einverständniserklärungen werden sicher vor dem Zugriff Dritter aufbewahrt.
Für die Unterstützung bei dem Vorhaben wäre ich sehr dankbar, bedanke mich im Voraus und stehe bei Rückfragen sowie auch für eine Rückmeldung gerne zur Verfügung.

Mit freundlichen Grüßen
Julia Eckhard, Marc Rodemer

Pseudonymisierung

Die Aufzeichnung und Auswertung der Daten erfolgt im IPN Kiel bzw. der JLU Gießen unter Verwendung eines persönlichen Codewortes, das ich selbst erstellt habe. Das Codewort ist so aufgebaut, dass niemand von meinem Codewort auf meine Person rückschließen kann, auch das Projektteam nicht. Ich selbst kann mein Codewort aber jederzeit rekonstruieren, wenn ich danach gefragt werde und es vergessen haben sollte.

Dies sind die Bestandteile des Codeworts:

- Die beiden letzten Buchstaben des Geburtsnamens Ihrer Mutter
- Die Anzahl der Buchstaben des (ersten) Vornamens Ihrer Mutter
- Die beiden letzten Buchstaben des (ersten) Vornamens Ihres Vaters
- Ihr eigener Geburtstag (nur der Tag, nicht Monat und/oder Jahr).

Einverständniserklärung

Ich erkläre mich hiermit damit einverstanden, dass ich an der vom Institut für Didaktik der Chemie der Justus-Liebig-Universität und vom Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN) durchgeführten wissenschaftlichen Untersuchung im Rahmen des Projekts EYEOC teilnehme. Die Studienleitung hat mich schriftlich und umfassend über das wissenschaftliche Untersuchungsvorhaben informiert. Ich erkläre mich damit einverstanden, dass erhobene personenbezogene Daten im Rahmen der genannten wissenschaftlichen Untersuchung verarbeitet werden dürfen (Tonaufnahmen, Filmaufnahmen der Hände und Unterarme, Alter, Geschlecht, Studiengang, Semester, Abiturnote, OC-1 Note). Das Informationsschreiben zum Datenschutz gemäß Art. 13 DSGVO habe ich zur Kenntnis genommen.

Ort, Datum Unterschrift

Informationspflichten gemäß Artikel 13 DSGVO

Durchführende Institutionen	Justus-Liebig-Universität, Institut für Didaktik der Chemie, Heinrich-Buff-Ring 17, 35392 Gießen
	Leibniz-Institut für die Pädagogik der Naturwissenschaften und Mathematik (IPN), Didaktik der Chemie, Olshausenstr. 62, 24118 Kiel
Projektleitung	Prof. Dr. Nicole Graulich (Tel. 0641 99 34601,
	E-Mail: Nicole.Graulich@didaktik.Chemie.uni-giessen.de)
	Dr. Sascha Bernholt (Tel.: 0431-880 3160,
	E-Mail: bernholt@ipn.uni-kiel.de)
Ansprechpartner	Julia Eckhard, (Tel. 0641-99 34631,
	E-Mail: Julia.Eckhard@didaktik.Chemie.uni-giessen.de)
	Marc Rodemer (Tel.: 0431-880 6416,
	E-Mail: rodemer@ipn.uni-kiel.de)
Datenschutzbeauftragter	Dr. Tim Höffler (Tel.: 0431-880 4834,
	E-Mail: hoeffler@ipn.uni-kiel.de)

Zweck für die Verarbeitung personenbezogener Daten und Rechtsgrundlage der Verarbeitung

Die erhobenen Daten werden ausschließlich zu wissenschaftlichen Zwecken verarbeitet. Interviews werden transkribiert. Die Teilnahme an der wissenschaftlichen Untersuchung ist grundsätzlich für alle Beteiligten freiwillig, aus einer Nichtteilnahme erwachsen keine Nachteile. Die Teilnehmenden geben ihre schriftliche Einwilligung zu der Verarbeitung der sie betreffenden personenbezogenen Daten für den o.a. Zweck, wodurch die Verarbeitung der personenbezogenen Daten gemäß Artikel 6 Absatz 1 Buchstabe a DSGVO rechtmäßig wird.

Speicherung und Verarbeitung personenbezogener Daten

Die personenbezogenen Daten werden gemäß den Empfehlungen der Deutschen Forschungsgemeinschaft (DFG) für mindestens zehn Jahre in gesicherten Systemen in Deutschland gespeichert. Die Daten werden gegen jeden unzulässigen Zugriff technisch geschützt. Die Verarbeitung personenbezogener Daten erfolgt ausschließlich auf institutsinternen und gegen jeden unzulässigen Zugriff technisch geschützten Geräten. Es findet kein Transfer der Daten an Dritte, in ein Nicht-EU/EEC Land oder internationale Organisationen statt. Eine Nachnutzung der Daten im Rahmen der wissenschaftlichen Forschung kann jedoch unter Umständen gestattet werden, sofern die hier bekannten Grundsätze der Datennutzung, Speicherung und Verarbeitung nicht verletzt werden.

Recht auf Auskunft über personenbezogene Daten (Artikel 15 DSGVO) sowie Berichtigung, Löschung, Einschränkung der Verarbeitung oder Widerspruch gegen die Verarbeitung personenbezogener Daten (Artikel 16-19, 21 DSGVO)

Für die Teilnehmenden besteht ein Recht auf Auskunft über die sie betreffenden personenbezogenen Daten sowie auf Berichtigung, Löschung, Einschränkung der

Verarbeitung sowie Widerspruch gegen die Verarbeitung der sie betreffenden personenbezogenen Daten. Hierzu wenden sich Teilnehmende unter Angabe ihres Codes an die Studienleitung. Durch die Übersendung des Codes ist kurzfristig eine personenbezogene Zuordnung des Datensatzes für den Zweck der Löschung möglich. Durch die Übersendung einer entsprechenden Anfrage erklären sich die Teilnehmenden mit diesem Umstand einverstanden.

Recht auf Datenübertragbarkeit (Artikel 20 DSGVO)
Die Teilnehmenden haben das Recht, die sie betreffenden personenbezogenen Daten zu erhalten und an Dritte zu übermitteln. Zudem haben sie das Recht zu erwirken, dass die sie betreffenden personenbezogenen Daten direkt von einem Verantwortlichen einem anderen Verantwortlichen übermittelt werden. Hierzu wenden sich Teilnehmende unter Angabe ihres Codes an die Projektleitung. Durch die Übersendung des Codes ist kurzfristig eine personenbezogene Zuordnung des Datensatzes für den Zweck der Löschung möglich. Durch die Übersendung einer entsprechenden Anfrage erklären sich die Teilnehmenden mit diesem Umstand einverstanden.

Recht auf Widerruf der Einwilligung
Die Teilnehmenden können ihre Einwilligung zur Verarbeitung sie betreffender personenbezogener Daten sowie generell zur Teilnahme an der wissenschaftlichen Untersuchung bis zur Vernichtung sämtlicher erhobener Daten unter Angabe des Codes an die Projektleitung widerrufen. Bei der wissenschaftlichen Untersuchung selbst können die Teilnehmenden ihre Teilnahme jederzeit ohne Angabe von Gründen verweigern, abbrechen oder auch Fragen auslassen. Durch die Übersendung des Codes ist kurzfristig eine personenbezogene Zuordnung des Datensatzes für den Zweck der Löschung möglich. Durch die Übersendung einer entsprechenden Anfrage erklären sich die Teilnehmenden mit diesem Umstand einverstanden.

Recht auf Beschwerde bei einer Aufsichtsbehörde
Die Teilnehmenden haben ein Recht auf Beschwerde bei der entsprechenden Aufsichtsbehörde.
Der Hessische Beauftragte für Datenschutz und Informationsfreiheit, Postfach 3163, 65021 Wiesbaden, poststelle@datenschutz.hessen.de
oder
Unabhängiges Landeszentrum für Datenschutz Schleswig-Holstein, Holstenstraße 98, 24103 Kiel, mail@datenschutzzentrum.de

10.6. Second Study: Guidelines for the Interview and Interview Protocol

Interviewleitfaden

Begrüßung

Formalia

- Grund der Studie: Wir wollen die Erklärungen von Studierenden beim Umgang mit organischen Reaktionsmechanismen untersuchen.
  - **Einverständniserklärung** unterschreiben lassen, dass erhobene Daten für Forschungszwecke verwendet werden dürfen und ggf. in der Lehre eingesetzt werden dürfen.
- Demografische Angaben
  - Kennung: _ _ _ _ _ _ _ _ (z.B. FG04RK23)
  - Alter:
  - Geschlecht:
  - Studienfächer:
  - Semesterzahl:
  - OC besucht j/n
  - OC bestanden j/n:
  - An vergleichbarer Studie teilgenommen?:
  - Möglichkeit der Teilnahme an Interventionsvorlesung (11.06.19)? j/n?
- Vorbereitung zum Prä/Post-Interview
- Handy aus?

Erwartungen:

- Im Prä-/ und Post-Interview gibt es verschiedene Aufgaben, die Inhalte der Studie aufgreifen und uns dabei helfen sollen, nachzuvollziehen wie sinnvoll unsere Intervention/unser Material war
- Es werden Fragen gestellt, die helfen sollen deine Denkprozesse und im Allgemeinen Denkprozesse von Studierenden nachzuvollziehen, damit wir Implikationen für die Lehre finden können.
- Die Aufgaben und Fragen dienen dazu dich besser zu verstehen, nicht deine Leistung abzuprüfen. Die Inhalte der Studie/des Interviews werden anonymisiert und sind nicht auf deine Person zurückführbar. Wir sind zur Verschwiegenheit verpflichtet (siehe **Datenschutzerklärung**).

Interviewprotokoll

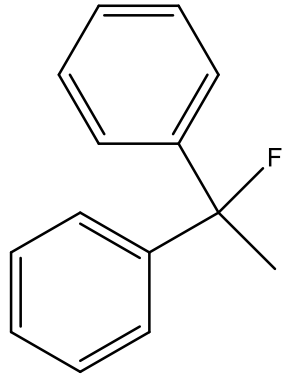
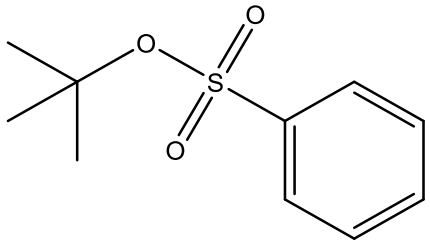
Situation	Reaktion

• Ungenaue Formulierung
• Austauschbare Phrasen:
  ○ „energetisch günstiger“
  ○ „stabiler“
	Was meinst du genau damit?
	Kannst du mir das genauer erklären?
	Was ist mit „[stabiler]“ gemeint?

Falsche Äußerungen	Achtung: Nicht beeinflussen, keine Suggestion, nur nachfragen, z.B. Was meinst du damit?
Nennung einer impliziten Eigenschaft	Von welchem Teil der Struktur hast du das abgeleitet? Wie kommst du darauf, dass das für diese Reaktion relevant ist? Warum erscheint dir das hier wichtig? Woran machst du das fest?
Pause	Was irritiert dich? Warum schwankst? Sag mal, woran du jetzt denkst. [Meta-Ebene anbieten] Ich weiß, du hast mir das jetzt schon einmal erläutert. Aber bitte hilf mir, das besser zu verstehen, wenn du dass jetzt noch einmal beschreibst.
Vorgehensweise erforschen?	Könntest du es einem Kommilitonen/mir erklären, wenn ich es nicht verstehe? Wie würdest du es jemanden erklären, der es nicht versteht?
Umgangssprache, Vermenschlichung „Leichter“, „Umklappen“, „besser“	Fragen, ob die gerade gesagte Aussage generalisierbar ist. Erinnerst du dich an andere Reaktionen, bei denen das wichtig ist?
Schluss	Hast du noch etwas vergessen? Möchtest du noch was ergänzen? Wenn nicht, gehen wir zur nächsten Aufgabe.

Interviewaufgaben

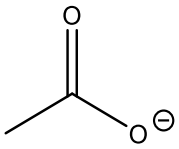
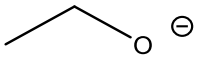
1. Zwei Kommilitonen aus dem OC-1 Kurs streiten sich welches das **bessere Substrat** für eine nukleophile Substitutionsreaktion erster Ordnung ist. Welches der beiden Moleküle würdest du präferieren? **Begründe** mir doch bitte mal, wer ein geeigneteres Substrat vorgeschlagen hat.

Laura	Michael
	

- *Wie sähe das Molekül, denn aus, wenn XY/die Abgangsgruppe das Molekül verlässt? (Zeichnen lassen)*
- *Was ist unterschiedlich im Vergleich zu Y/X? (Zeichnen lassen)*
- *Woran machst du fest, dass es das bessere Substrat ist? (Auf AG und Substrat-Grundgerüst eingehend?)*
- *Wie würdest du jemandem erklären was eine gute/schlechte Abgangsgruppe ist?*
- *Wie würdest du jemandem erklären was eine gutes/schlechtes Substrat ist?*

- ***Prompts,*** wenn Studis in diese Richtung gehen (keine Instruktion beim Pre-Interview!)
- *Was bedeutet gut/tertiär/stabiler?*
- *Was heißt denn „positive Ladung" ist stabiler? Kannst du mir das mal zeichnen?*
- *Was unterscheidet die beiden Moleküle voneinander?*
- *Worin liegt denn der Unterschied zwischen den Aromaten und den Methyl-Gruppen?*
- *Woran machst du fest, dass es das bessere Substrat ist? (Auf AG und Substrat-Grundgerüst eingehend?)*
- *Wie würdest du jemandem erklären was eine gute/schlechte Abgangsgruppe ist?*
- *Woran siehst du das an der Repräsentation/der Darstellung?*
- *Wenn dir ein Kommilitone sagt, dass er das nicht versteht, wie würdest du es ihm erklären?*

2. Wenn du dich wieder entscheiden müsstest, ob Laura oder Michael das **bessere Nukleophil** für eine nukleophile Substitutionsreaktion zweiter Ordnung ausgesucht haben, für welches würdest du dich entscheiden? **Begründe** mir das bitte mal.

Laura	Michael
	

- *Woran machst du fest, dass es das bessere Nukleophil ist?*
- *Wie würdest du jemandem erklären was eine gutes/schlechtes Nukleophil ist?*

Prompts, wenn Studis in diese Richtung gehen (keine Instruktion beim Pre-Interview!)

- *Wie sähe das Molekül, denn aus, wenn die Elektronenpaare umklappen? (Zeichnen lassen)*
- *Was bedeutet gut/tertiär/stabiler?*
- *Aber die beiden Moleküle sehen sich doch ähnlich, mit dem O-Minus? Worin unterscheiden sie sich?*
- *Wie würdest du jemandem erklären was ein gutes/schlechtes Nukleophil ist?*
- *Woran siehst du das an der Repräsentation/der Darstellung?*
- *Wenn dir ein Kommilitone sagt, dass er das nicht versteht, wie würdest du es ihm erklären?*

3.

a) Du lässt das von dir ausgewählte Nukleophil aus der vorherigen Aufgabe mit **1-Chlorpropan** reagieren. **Zeichne** die Reaktion. **Beschreibe** mir den ablaufenden Prozess.

- *Warum läuft es denn nach S_N1/S_N2?*
- *Warum greift das Nukleophil genau dort an?*
- *Was bewegt das Nukleophil anzugreifen?*

Prompts, wenn Studis in diese Richtung gehen (keine Instruktion beim Pre-Interview!)

- *Ein Kommilitone fragt dich, warum die Reaktion abläuft. Erkläre ihm dies bitte in deinen eigenen Worten.*

b) Was könntest du an den Edukten verändern, damit die Reaktion nach S_N2 nicht mehr abläuft?

- *Proband: lässt es z.B. nach SN1 ablaufen: Welche anderen Faktoren könnte man noch verändern?*
- *Wenn auf Konz./Temp. etc eingegangen wird: Was würdest du strukturell ändern?*
- *Warum würdest du das nehmen?*
- *Worin liegt der Unterschied zwischen dem Gezeigten → Nukleophil/Substrat/Abgangsgruppe*

- *Was macht das für einen Unterschied?*
- *Welchen Effekt hat das von dir Überlegte nun auf die Reaktion? Schneller/langsamer? S_N1/S_N2?*
- *Welche anderen Faktoren könnte man noch verändern?*

c) Wenn du jetzt deine gezeichnete Reaktion mit der unteren Reaktion vergleichen würdest, welche der beiden Reaktionen wäre **schneller**? Du siehst ja, das Substrat ist gleich, aber das Nukleophil ist ein anderes (*bisschen anleiten hier*). Nimm dir erstmal Zeit und schaue es dir an.

- *Wenn ich jetzt auf dich zukommen würde und ich sagen würde: „ich verstehe nicht, wie ich das beantworten soll." Wie würdest du vorgehen?*

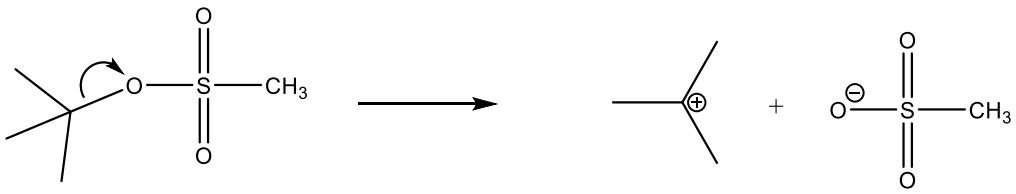
Prompts, wenn Studis in diese Richtung gehen (keine Instruktion beim Pre-Interview!)

- *Woran machst du fest, dass Reaktion XY die schnellere ist?*
- *Was bedeutet gut/besser/schneller/stabiler?*

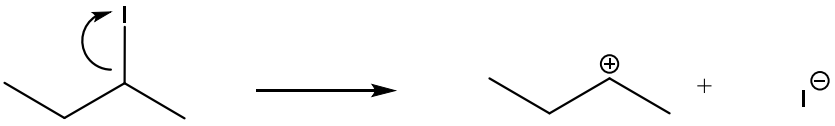
4.

a) Du bist jetzt ja schon im Erklären und Begründen geübt. Hier haben wir noch so einen Fallvergleich von zwei Reaktionen. Kannst Du auch hier entscheiden, welche der beiden Reaktionen schneller ist?

A



B



Beschreibe mir wie du so einen Fallvergleich lösen würdest.

Prompts, wenn Studis in diese Richtung gehen (keine Instruktion beim Pre-Interview!)

- *Woran machst du fest, dass Reaktion XY die schnellere ist?*
- *Was bedeutet gut/besser/schneller/stabiler?*

Post-Interview Zusatz:

Einstieg:

- Was ist dir [von der Intervention] im Gedächtnis geblieben?
- War dir etwas neu?

- Wie sahen Videos aus, die du gesehen hast? (Gruppenzuordnung herausfinden)
    - Dynamic: Static: No Cue:

- Was hättest du dir gewünscht bei einem Erklärvideo über nukleophile Substitutionsreaktionen? Hätten wir etwas anders machen sollen?

- Würdest du sagen das Anschauen hat dir etwas gebracht/war hilfreich? Was hätte dir geholfen noch mehr zu lernen?
- Was hast du aus den Videos zusätzlich mitgenommen?

Visualisierung:

- Wie war dein Eindruck beim Anschauen? Schwergefallen zu folgen – leicht?
- No Cue: Konntest du das, was gesagt wurde den Strukturen zuordnen?
- Dynamic/Static Cue:
- Wie haben dir die Hervorhebungen gefallen?
- Wie hast du die Verknüpfung mit der Tonspur für wahrgenommen?
- Was hätten wir besser machen können?

Verbalerklärung:

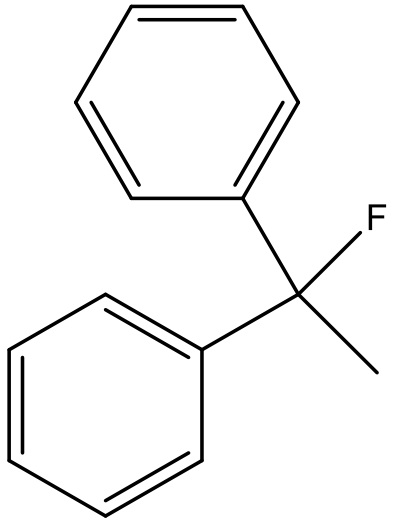
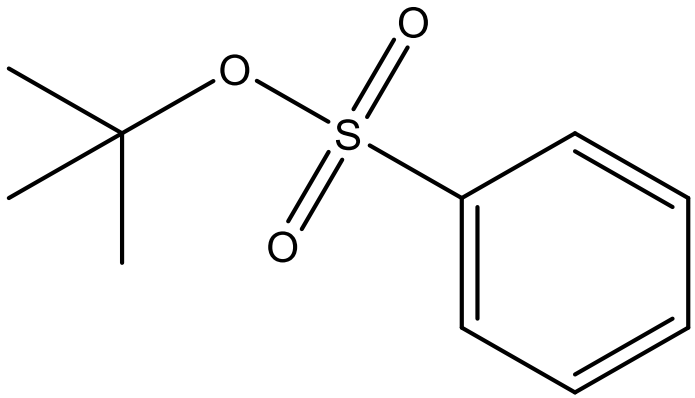
- Wie hat dir die Tonspur/das Gesagte gefallen?
- Würdest du sagen das Anschauen/das Gehörte hat dir etwas gebracht/war hilfreich? Was hätte dir geholfen noch mehr zu lernen?
- Wie hast du die Verknüpfung mit Visualisierung wahrgenommen?

- Wenn du jetzt nochmal alle 3 Videos in deinen Kopf rufst, kannst du dich an eine allgemeine Vorgehensweise erinnern?
- Möchtest du noch etwas ergänzen?
- Wie hat es dir allgemein gefallen?

10.7. Second Study: Tasks in the Interview

Please note that only part of the data from the students' solutions was used in this dissertation.

Aufgabe 1)

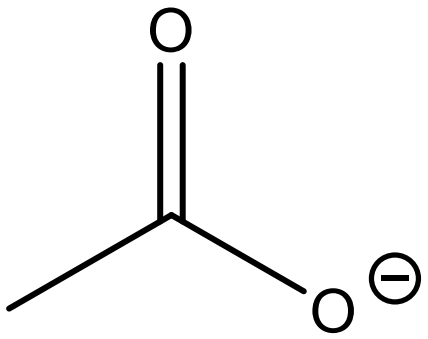
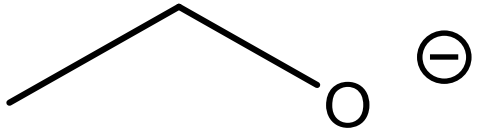
Laura	Michael
	

Für wen hast du dich entschieden?

Laura ☐

Michael ☐

Aufgabe 2)

Laura	Michael
	

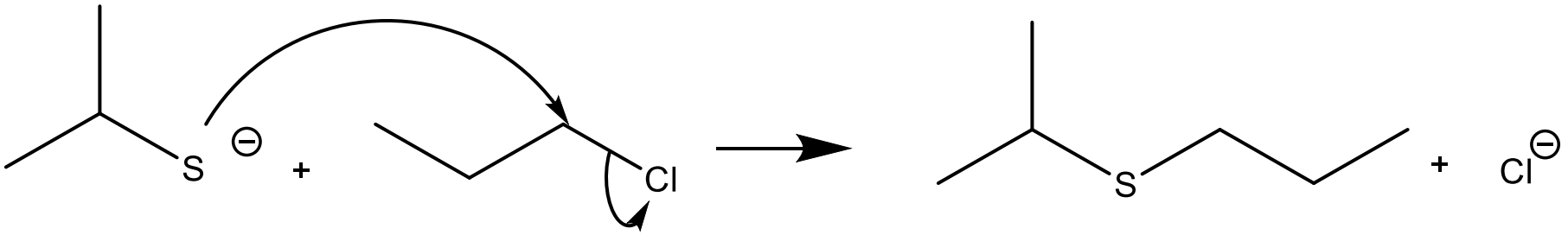
Für wen hast du dich entschieden?

Laura ☐

Michael ☐

Aufgabe 3 a)

Aufgabe 3 c)



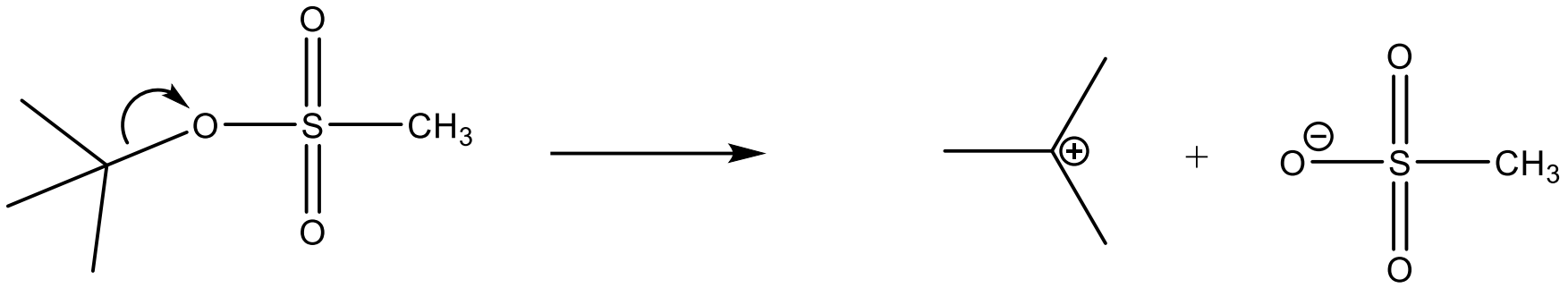
Für welche Reaktion hast du dich entschieden?

Mit Sauerstoff-Nukleophil ☐

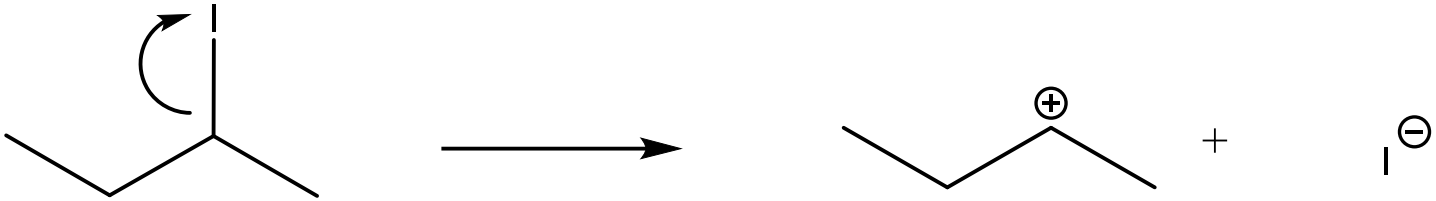
Mit Schwefel-Nukleophil ☐

Aufgabe 4 a)

A



B

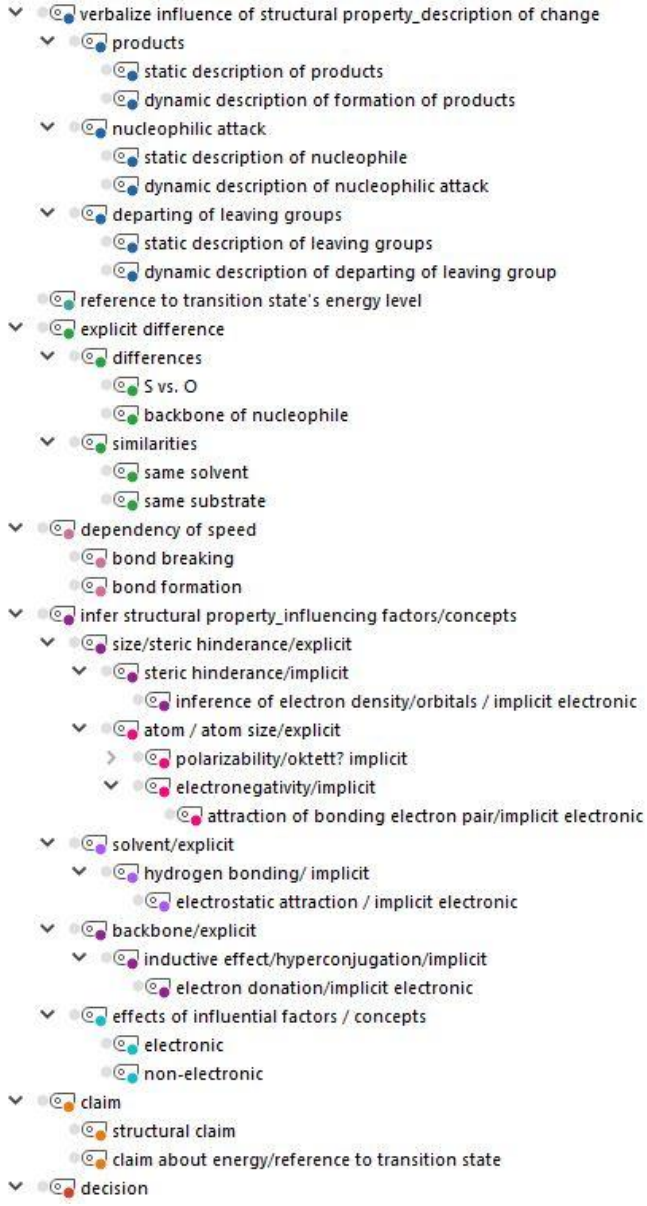


Für welche Reaktion hast du dich entschieden?

A ☐

B ☐

10.8. Coding System Used in the Second Study



10.9. Participants Original Quotes and Their English Translation

The translation of the quotes from the participants is presented in the following. In cases where the participants' original responses in German were in some way non-standard (e.g., in expression, word order, etc.), but the direct translation into English was still interpretable, the non-standard grammar and wording was left as intact as possible in the translation. This was done in order not to extend the information of the participants' responses beyond what they had expressed and to ensure the representativeness of the meaning.

Study 1/Paper 1:

Text passage	German transcript	English translation of the transcript
Results and discussion, p. 86	Prof. Franklin: SN1-Substitution. Tertiäres Substrat versus zweimal benzylisch tertiäres Substrat. B ist um Größenordnungen schneller.	Instructor Franklin: S_N1 substitution. Tertiary substrate versus twice benzylic tertiary substrate. B is faster by orders of magnitude. (Task 4, expert frame)
Results and discussion, p. 86	Prof. Evans: Ja, es geht um die Abspaltung von einer Abgangsgruppe und dann machen wir ein sekundäres und tertiäres Substrat. Und das tertiäre wird ziemlich sicher besser gehen, weil es besser stabilisiert ist durch induktive Effekte.	Instructor Evans: Yes, it's about splitting off from a leaving group and then a secondary and tertiary substrate form. In addition, the tertiary will almost certainly go better because it is better stabilized through inductive effects. (Task 1, expert frame)
Results and discussion, p. 87	Prof. Davis: Die zweite Reaktion verläuft schneller. Das liegt an der Stabilität des entstehenden kations. Das Biphenylsubstituierte Kation ist stabiler als das Tertiärbutylkation, was wir in Reaktion A sehen. Und das liegt an den beiden Phenylsubstituenten. Die tragen durch die Elektronendichte der p-Orbitale dazu bei, dass dieses Kation sehr stabil ist. Das leere p-Orbital dieses Kations kann mit den p-Orbitalen beider Phenylringe in Resonanz gehen und so wird, wenn man so will, positive Ladung über 13 C-Zentren delokalisiert. Dann hat jeder nur noch ein 13tel der Elektronendefizitlast zu tragen. Ja das macht die besondere Stabilität dieses Kations aus.	Instructor Davis: […] The second reaction is faster. This is due to the stability of the generated cation. The biphenyl substituted cation is more stable than the tertiary butyl cation, which we see in reaction A. And this is due to the two phenyl substituents. They contribute to the stability of this cation by donating electron density of the p-orbitals. The empty p-orbital of this cation [in B] can overlap with the p-orbitals of both phenyl rings and thus positive charge is delocalized over 13 C-centers [carbon atoms]. Then each of them [the carbon atoms] has to carry only a 13th of the electron deficit load. Yes, this is what makes this cation so stable. […] (Task 4, teaching frame, excerpt)
Results and discussion, p. 87-88	Prüf. Müller: […] im einen Falle ist es ein tertiäres Carbeniumion, was sich ausbildet, im oberen Beispiel, im unteren Beispiel ein sekundäres Carbeniumion. Das ist also der Unterschied. Also die Frage, welches von beiden Carbeniumionen sich schneller bildet, hängt zusammen mit der Stabilität. Je stabiler das Carbeniumion ist, desto schneller wird es sich auch bilden. Und	Instructor Miller: […] in one case it's a tertiary carbocation that forms, in the upper example, in the lower example it's a secondary carbocation. So, that's the difference. So the question of which of the two carbocations forms faster is related to stability. The more stable the carbocation, the faster it will form. And on the grounds of the +I effect of the

	anhand des +I-Effektes der Methylgruppen, der ja im oberen Falle stärker ist als im unteren Falle, weil wir oben drei Methylgruppen haben, die einen +I-Effekt ausüben, unten nur zwei Methylgruppen mit +I-Effekt, können wir sehen eben, das obere Carbeniumion ist stabiler und wird sich entsprechend auch schneller bilden.	methyl groups, which is stronger in the upper case than in the lower case, because we have three methyl groups at the top, which have a +I effect, and only two methyl groups with a +I effect at the bottom, therefore the upper carbocation is more stable and will also form faster. (Task 1, teaching frame)
Results and discussion, p. 88	Prof. Evans: […] Durch die induktiven Effekte, die die drei Methylgruppen ausüben, was stärker wirkt als im unteren Fall mit den zwei Methylgruppen, haben wir einen schnelleren Reaktionsverlauf im Falle eines tertiären Systems. […]	Instructor Evans: […] Due to the inductive effects by the three methyl groups, which have a stronger impact than in the lower case with the two methyl groups, we have a faster reaction progression in the case of a tertiary system. […] (Task 1, teaching frame)
Results and discussion, p. 89	Prof. Robinson: Also das Untere ist schneller, weil wir haben hier zwei unterschiedliche Abgangsgruppen. Bei dem einen ist das Amin und dann ist das Amid, was rausgeht. Bei dem anderen ist es das Mesylat was rausgeht und beim Mesylat sind natürlich die, ist die negative Ladung, also die Abgangsgruppe wesentlich besser stabilisiert und das Amid eben nicht.	Instructor Robinson: So the lower one is faster because here we have two different leaving groups. One is an amine and then we have the amide that leaves. In the other one, it is the mesylate that leaves and in the mesylate, of course… well the leaving group is much better stabilized and the amide is just not [stabilized]. (Task 2, expert frame)
Results and discussion, p. 89	Prof. Robinson: Genau. Wenn wir hier die Reaktionen vergleichen, ist der Unterschied, die Abgangsgruppe. Wir haben oben einfach ein Amin, während wir unten ein Mesylat haben. Das heißt, auch wenn beide Reaktionen nach S_N2 gehen, schauen wir uns die unterschiedliche Qualität der Abgangsgruppe an und damit schauen wir uns an, wie stabilisiert die Abgangsgruppe ist, wenn sie dann abgespalten ist. Das heißt, wir haben einmal oben das Amid, also NH_2 minus, während wir unten eben das Mesylat haben. Die negative Ladung kann im unteren Fall eben über alle drei Sauerstoffe verteilt werden, indem wir einfach die Elektronenpaare umklappen. Das heißt, wir haben einen starken mesomeren Effekt auch und wie Sie wissen, sind geladene Spezies, je weiter man die über oder je mehr Atome man sie verteilen kann, desto günstiger ist es.	Instructor Robinson: Right. If we compare the reactions here, the difference is the leaving group. We simply have an amine at the top [reaction A] and mesylate at the bottom [reaction B]. This means that even if both reactions run by a S_N2 mechanism, we compare the different quality of the leaving group and thus we see how stabilized the leaving group is when it is split off. This means that we have the amide at the top [reaction A], accordingly, NH_2 minus, while we have the mesylate at the bottom [reaction B]. In the lower case, the negative charge can be distributed over all three oxygen atoms by simply flipping over the electron pairs. That means there is a strong mesomeric effect present and as you know, charged species are the more you can distribute their charge or the more atoms you can distribute it to, the more favorable. […] (Task 2, teaching frame, part 1 of his explanation)
Results and discussion, p. 90	Prof. Robinson: Das kann man auch direkt korrelieren, mit dem pKS-Wert. Das heißt, je stärker die korrespondierende der Säure zu dem Anion ist, desto besser ist das Anion als Abgangsgruppe. Und wenn Sie jetzt einmal sich den pKS-Wert von dem Amin vor Augen halten und den vergleichen mit der entsprechenden Sulfonsäure, dann	Instructor Robinson: This can also be directly correlated with the pK_a value. That means, the stronger the corresponding acid to the anion, the better the anion can be considered as leaving leaving group. And if you now look at the pK_a value of the amine and compare it with the corresponding

	würden Sie sofort sehen, dass das Amin wesentlich schwächer sauer ist, weil eigentlich reagieren Amine ja nach allem als Base und daraus können Sie ableiten, dass das Mesylat die wesentlich bessere Abgangsgruppe ist und damit in B schneller gehen sollte.	sulfonic acid then you would immediately see that the amine is much less acidic, because amines react as a base after all and from this you can deduce that mesylate is the better leaving group and should be faster in B. (Task 2, teaching frame, part 2 of his explanation)
Results and discussion, p. 90	Prof. Carter: In beiden Fällen handelt es sich um SN2-Reaktionen, unzweifelhaft. Das gute Nukleophil substituiert zwei in beiden Fällen gute Abgangsgruppen. Die untere Abgangsgruppe Trifluoracetat ist allerdings noch ein bisschen schlechter als die bere Abgangsgruppe, das Trifluorsulfonat. Das hängt damit zusammen, dass das Trifluorsulfonation noch besser stabilisiert ist als das Trifluoracetation und insofern die schwächere Base ist. Umgekehrt ist Trifluoressigsäure eine stärkere Säure als Trifluor äh entschuldigung, ist Trifluormethylsulfonsäure, also die korrespondierende Säure des oberen, der oberen Abgangsgruppe, die stärkere Säure als Trifluoressigsäure.	Instructor Carter: In both cases, the reactions are S_N2 reactions, without any doubts. The good nucleophile substitutes two good leaving groups. However, the lower leaving group trifluoroacetate is still a bit worse than the upper leaving group, the trifluorosulfonate [trifluoromethanesulfonate]. This is because the trifluorosulfonate ion [trifluoromethanesulfonate] is even better stabilized than the trifluoroacetate ion and is therefore the weaker base. Conversely, trifluoroacetic acid is a stronger acid than trifluoromethanesulfonic acid, so the corresponding acid of the upper leaving group, is the stronger acid than trifluoroacetic acid. (Task 3, expert frame)
Results and discussion, p. 90	Prof. Carter: Die obere Reaktion ist deswegen schneller, weil das, sich bildende / also die bildende / die sich bildende Abgangsgruppe durch Mesomerie besser stabilisiert als im unteren Fall. Im oberen Fall kann man drei Grenzformeln formulieren. Im unteren Fall wären nur zwei. Und die Möglichkeit rationale Grenzformeln zu formulieren geht tatsächlich zusammen, in aller Regel, mit Teilchenstabilität. Prüfen kann man das, in dem man die Acidität der korrespondierenden Säuren nachschaut. Die korrespondierende Säure im oberen Fall wäre ja die Trifluormethansulfonsäure. Und das ist eine stärkere Säure als die Trifluoressigsäure. So dass also wegen der grundsätzlich geringeren Basizität und höheren Stabilität der oberen Abgangsgruppe die obere Reaktion schneller verläuft.	Instructor Carter: The upper reaction is faster because the forming negatively charged leaving group is better stabilized via resonance than in the lower case. In the upper case, you can formulate three contributing structures [resonance structures]. In the lower case, there would only be two. And the possibility to formulate contributing structures which actually goes hand in hand, generally speaking, with stability of entities. One can check this by looking up the acidity of the corresponding acids. The corresponding acid in the upper case would be trifluoromethanesulfonic acid. And this is a stronger acid than trifluoroacetic acid. So, because of the fundamentally lower basicity and higher stability of the upper leaving group, the upper reaction is faster. (Task 3, teaching frame)
Results and discussion, p. 90	Prof. Franklin: […] Die Fähigkeit eine gute Abgangsgruppe zu sein, korreliert mit der Säurestärke. Ammoniak ist eine Base, also wissen wir, eine ganz schlechte Säure. Mehtansulfonsäure, wie es der Name sagt, ist eine echte Säure, das heißt die stärkere Säure ist die Methansulfonsäure, damit ist das die bessere Abgangsgruppe. Bedeutet die Reaktion 2, B, muss deutlich schneller verlaufen.	Instructor Franklin: […] The ability to be a good leaving group correlates with acid strength. Ammonia is a base, so we know, a very bad acid. Methanesulfonic acid, as the name implies, is a real acid, which means the stronger acid is methanesulfonic acid, so that is the better leaving group. Which means reaction 2, B, is got to go much faster. (Task 2, teaching frame)

Results and discussion, p. 91	Prof. Schmidt: wenn sie nach der Schnelligkeit der Reaktion fragen. Dann müsste man mit den Aktivierungsenergien arbeiten und ich kann nicht einfach sagen "es wird das stabilere Kation gebildet, deshalb reagiert es schneller." Also es kommt in welcher / in welchem Level ich mich befinde beim Erklären. Also in der Schule würde man das sicherlich so erklären. Ähm. In OC1 würde ich mich Energiediagrammen arbeiten, um dann halt nach dem Hammond-Postulat für diesen exothermen Schritt den Übergangszustand mit dem Produkt, in diesem Fall dem Kation, korrelieren.	Instructor Smith: If you ask about the speed of the reaction, then you would have to work with the activation energies and I cannot just say 'the more stable cation is formed, therefore it reacts faster'. It depends on which level of explanation I adapt. So, in school, that is certainly how you would explain it. Um. In an introductory Organic Chemistry course, I would work with energy diagrams to correlate the transition state with the product, in this case [referring to task 1] the cation, according to the Hammond postulate for this exothermic step.
Results and discussion, p. 91	Prof. Jones: Weiter. (…) Hier unterscheidet sich wieder die Abgangsgruppe. Einmal ein Trifluoracetat im Fall B. Und im Fall A ein Trifluormethansulfonat. Ähm. Beides wieder S_N2-Reaktionen. Das Trifluormethansulfonat, ähm, ist die bessere Abgangsgruppe als das Trifluoracetat. Und deshalb wird A schneller verlaufen als B.	Instructor Jones: Here the leaving group differs. Once a trifluoroacetate in case B. And in case A a trifluoromethanesulfonate. Both are S_N2 reactions. The trifluoromethanesulfonate is the better leaving group than the trifluoroacetate. And therefore, A will proceed faster than B. (Task 3, expert frame)
Results and discussion, p. 91	Prof. Jones: Weiter. Hier haben wir einen Fall eines primären Substrates mit zwei unterschiedlichen Abgangsgruppen, das Nukleophil ist wieder gleich, heißt, die Abgangsgruppe ist einmal ein Sulfonat und einmal ein Carboxylat, die Reste mit der CF_3-Gruppe sind auch noch gleich, das heißt, wir unterscheiden hier de facto zwischen Sulfonat und Carboxylat. Sulfonat ist das deutlich stabilere Anion und die bessere Abgangsgruppe und das heißt, der Fall A ist rascher als der Fall B.	Instructor Jones: Here we have a case of a primary substrate with two different leaving groups, the nucleophile is the same, the leaving group is once a sulfonate and once a carboxylate, the residues with the CF_3-group are also still the same, which means we have to distinguish between sulfonate and carboxylate. Sulfonate is the clearly more stable anion and the better leaving group and that means that case A is faster than case B. (Task 3, teaching frame)
Results and discussion, p. 93	Prof. Lewis: Wir sehen zwei Reaktionen, bei der ein Jodid ein Alkanfall ist, unter Ausbildung eines positiv geladenen Kohlenstoffatoms.	Instructor Lewis: We have two reactions, in which an iodide leaves an alkane, forming a positively charged carbon atom. […] (Task 1, expert frame, description of the process)
Results and discussion, p. 93	Prof. Lewis: Unterschied ist, dass es einmal ein sekundäres, einmal ein tertiäres ist. Im oberen Fall ist die positive Ladung bedeutend besser stabilisiert als im unteren, der Rest ist gleich. Jodid, also ist das in dem Fall der einzige Unterschied und auch das Entscheidende, das Obere dürfte aufgrund der besseren Stabilität schneller gebildet werden.	Instructor Lewis: […] The difference is that it is a secondary and a tertiary [carbocation]. In the upper case, the positive charge is significantly better stabilized than in the lower one, the rest is the same. The upper one should be formed faster because of the better stability. (Task 1, expert frame, rationale)
Results and discussion, p. 93	Prof. Lewis: Es geht um die Abspaltung der jeweils identischen Abgangsgruppe Iodid aus einem Alkyl, einmal sekundär, einmal tertiär. Es entsteht ein energetisch deutlich höher liegendes Carbokation. Das heißt,	Instructor Lewis: It is about the separation of the identical iodide leaving group from an alkyl, one is secondary, one is tertiary. An energetically much higher carbocation

	das Carbokation ist dann eine Zwischenstufe, ein Zwischenprodukt.	is formed. This means that the carbocation is then an intermediate stage, an intermediate product. […] (Task 1, teaching frame, description of the process)
Results and discussion, p. 93	Prof. Lewis: Und betrachten wir nun zunächst einmal die Energie dieser beiden Zwischenprodukte:	Instructor Lewis: […] And now let us first consider the energy of these two intermediates: […] (Task 1, teaching frame, approach)
Results and discussion, p. 93	Prof. Lewis: Es ist eine Elektronenmangelverbindung, das heißt, die Stabilisierung erfolgt durch Reste, die in irgendeiner Form Elektronen liefern können, sei es durch Mesomerie oder induktive Effekte.	Instructor Lewis: […] It is an electron-deficient compound. In general, stabilization is achieved by residues that can supply electrons in some way; be it through mesomeric effects or inductive effects. […] (Task 1, teaching frame, general statement)
Results and discussion, p. 93	Prof Lewis: Mesomerie haben wir hier nicht, wir haben nur induktive Effekte durch die Methyl-Gruppen. Oben haben wir drei Methyl-Gruppen, die diese Elektronenmangelverbindung, diese positive Ladung stabilisieren könnten, unten nur zwei. […]	Instructor Lewis: […] We do not have mesomeric effects, we only have inductive effects through the methyl groups. Above we have three methyl groups, which could stabilize this electron deficiency compound, this positive charge, below we have only two. […] (Task 1, teaching frame, rationale)
Results and discussion, p. 93	Prof. Müller: […] um zu schauen, welche Reaktion schneller ist, uns auf die Qualität der Abgangsgruppe stützen..	Instructor Miller: Well, to determine which reaction is faster, we have to rely on the quality of the leaving group. […] (Task 2, teaching frame, approach)
Results and discussion, p. 93	Prof Müller: […]Und es ist so, dass eine Abgangsgruppe umso stabiler ist, umso besser ist, je besser sie die negative Ladung stabilisiert	Instructor Miller: […] And it is like this: the more stable a leaving group, the better the negative charge can be stabilized. […] (Task 2, teaching frame, general statement)
Results and discussion, p. 93	Prof. Müller: und das können Sie entweder daran ablesen, dass Sie sich die Struktur anschauen und erkennen […]	Instructor Miller: […] And you can tell this either by looking at the structure and recognizing that […] (Task 2, teaching frame, approach)
Results and discussion, p. 94	Prof. Müller: Das war jetzt ja eine sehr knappe Erklärung. Reicht Ihnen das? Also ich meine, ich würde jetzt / das wäre jetzt meine Erklärung für einen Kollegen sozusagen. Ich meine bei einem Studenten würde ich jetzt sagen: "Mh Sie sehen ja diesselbe Abgangsgruppe. Es handelt sich um eine SN1-Reaktion. Der erste Schritt ist der geschwindigkeitsbestimmende […] So das wäre jetzt die Erklärung für einen Studenten sozusagen im OC-1 Interviewer: Genau, das ist ja Block 2. [Erklären für Studierende]	Instructor Miller: That was a very brief explanation. Is that enough for you? So, I mean, that would now be my explanation for a colleague, so to speak. I mean to a student I would explain: 'You see the same leaving group. It is a S_N1 reaction [goes on more in depth with his explanation]'. So that would now be the explanation for a student, so to speak, in an Organic Chemistry beginner course. Interviewer: Exactly, that [explaining to a fictitious student] will take place in the next scenario.

Results and discussion, p. 94	Interviewer: […] es ist einfach nur Ihre Erklärung. Prof. Lewis: Okay. Aber ich habe trotzdem Zeit, mich drauf vorzubereiten, didaktisch sinnvoll. Interviewer: Genau. Es sind aber die gleichen Aufgaben wie eben. Prof. Lewis: Okay, klar. Trotzdem: Ich glaube, da habe ich sozusagen eher für mich gedacht, und nicht mir überlegt, wie ich sinnvoll da hinkomme. Okay. Interviewer: Natürlich. Also Sie haben alle Zeit der Welt.	Interviewer: […] now we go on with your explanation [in the teaching frame]. Instructor Lewis: Okay. But I still have time to prepare for it, to explain in a didactically meaningful way? Interviewer: Of course. But the task format is the same like before [in the expert frame]. Instructor Lewis: Okay, sure. Still, I think there [in the expert frame] I was thinking more for myself, so to speak, and not thinking about how to get there in a meaningful way. (Before starting the teaching frame)
Dissertation, Chapter 3.2.3.	Instructor Evans: Das heißt: Die Reaktivität für nukleophile Substitutionsreaktion nimmt grundsätzlich im Falle der SN1 von primär über sekundär zu tertiär zu.	Instructor Evans: […] That is, the reactivity for nucleophilic substitution reaction basically increases from primary to secondary to tertiary in the case of S_N1. (Task 1, expert frame, not mentioned in the paper)
Dissertation, Chapter 3.2.3.	Prof. Davis: Es geht alles immer nach dem Prinzip: Elektrophil reagiert mit Nukleophil. Und wenn das Elektrophil elektrophiler ist, dann geht die Reaktion schneller. Wenn das Nukleophil nukleophiler ist, geht die Reaktion schneller. Das kann man jetzt über alle Reaktionen, die wir hier jetzt in dem gleichen Kontext so vergleichen anwenden.	Instructor Davis: Everything is always based on the principle that an electrophile reacts with a nucleophile. And if the electrophile is more electrophilic, the reaction is faster. If the nucleophile is more nucleophilic, the reaction is faster. This can be applied to all the reactions we are comparing here in the same context. (Task 4, teaching frame, not mentioned in the paper).

Study 2/Paper 2:

Text passage	**German transcript**	**English translation of the transcript**
Dissertation, Chapter 3.3.2.	Emil: […] zumindest wurde es eben im Video so erklärt.	Emil […] it was explained in the video in such a way. Post-interview
Results and discussion, Figure 4, p. 2237	Isaac: So, dann würde ich erst mal schauen, wie das stabilisiert wird. Zum Beispiel würde ich mir die induktiven Effekte, habe ich ja eben schon gesagt, anschauen […].Ja, ich würde es jetzt hauptsächlich durch die induktiven Effekte begründen und würde jetzt also im zweiten Schritt halt auf die Elektronegativität schauen. Da wäre, meiner Meinung nach, Schwefel weniger elektronegativ als Sauerstoff. Und das würde eigentlich eher für den Sauerstoff sprechen. Aber hier würde ich denken, dass der Unterschied nicht so stark ist. Deswegen würde ich eher auf die induktiven Effekte achten, ja.	Isaac: I would focus on which of the two is more stable [points to the products of reaction A and B]. And then I would first go with, for example, something like inductive effects.[…] Yes, I would now mainly justify it by the inductive effects and would now look at the electronegativity in the second step. In my opinion, sulfur would be less electronegative than oxygen. And that would actually speak more in favor of oxygen. But here I would think that the difference is not so strong. So, I would rather look at the inductive effects, yes. Pre-interview
Results and discussion,	Isaac: Im Prinzip möchte ich ja die beiden Nucleophile vergleichen. Ich habe zwei Sachen, die ich dazu sagen kann.	Isaac: In fact, I would like to compare the two nucleophiles [points to ethanolate and 2-propanethiolate]. I have two things to say

Figure 4, p. 2237	Einmal ist Schwefel durch die größere …Dadurch, dass es einen größeren Radius hat und im Prinzip mehr Elektronen dort sind, also es ist ein größeres Atom, und interessant auch, mehr, ja, es sind mehr Elektronen vorhanden, dementsprechend auch lässt es sich leichter polarisieren. Im Vergleich zum Sauerstoff, wo die / Ja, also das heißt, hier (zeigt auf S-Atom) können zusätzlich noch die weiteren Außenelektronen sozusagen anders verteilt werden, sage ich jetzt mal. […] Also je näher es sozusagen an das Substrat herangeht, desto stärker wird das polarisiert und desto stärker wird es wieder angezogen. Und das ist halt so ein Effekt, der sich dann halt / also das verstärkt sich dann gegenseitig.	about this. One is sulfur by... the larger...by the fact that it has a larger radius and basically there are more electrons there, so it's a larger atom, and interesting also, more, yes, there are more electrons, accordingly also it's easier to polarize. Compared to oxygen, here [points to S atom 2-propanethiolate] additionally the outer electrons can be distributed differently, so to speak […] So, the closer it [points to S atom 2-propanethiolate] gets to the substrate the more polarized it gets and the more strongly it is attracted [to the electrophilic center]. And that's just such an effect that then just / so that then reinforces each other... Post-interview
Results and discussion, Figure 5, p. 2237	Emil: Ich kann jetzt O und S nicht so wirklich gut vergleichen, da sie ja auch untereinanderstehen, oder übereinander – wie auch immer. Deshalb würde ich jetzt als nächstes mal schauen, inwiefern das einen Unterschied macht, dass wir hier noch eine Methylgruppe dran haben, die hier an der Stelle nicht vorhanden ist. Doch, das gefällt mir eigentlich ganz gut, die Idee, weil dieses partiell eher positivere Kohlenstoffatom, hier an der Stelle, könnte diese Partialladung ja eher verteilen, auf zwei benachbarte Kohlenstoffatome. Und dieses Kohlenstoffatom könnte es nur auf ein benachbartes Kohlenstoffatom verteilen. Weswegen ich dann nach der Argumentation davon ausgehen würde, dass das hier stabiler ist. Und dementsprechend wäre das hier reaktionsfreudiger und das hier auch das bessere Nukleophil. Also das Nukleophil mit Sauerstoff ist das stärkere Nukleophil.	Emil: I can't really compare O and S very well now, because they are also underneath each other, or on top of each other - whatever. That's why the next thing I would look at is to what extent it makes a difference that we have an additional methyl group on it [points to 2-propanethiolate], which is not present here [points to ethanolate] at this point. Yes, I actually like this idea, because this partially more positive carbon atom, here at this position [points to C1 of 2-propanethiolate], could rather distribute this partial [positive] charge to two neighboring carbon atoms. And this carbon atom [points to C1 of ethanolate] could distribute it only to one neighboring carbon atom. Which is why, according to this line of argumentation, I would assume that this is more stable [points to 2-propanethiolate]. And accordingly, this would be more reactive [points to ethanolate] and this would be the better nucleophile [points to ethanolate]. Therefore, the nucleophile with oxygen is the stronger nucleophile. Pre-interview
Results and discussion, Figure 5, p. 2237	Emil: ist es hier (zeigt auf S-Atom des 2-Propylthiolats auf S.6) so, dass das S Minus reaktiver ist als das O Minus. Beide haben erstmal die gleiche Anzahl an Valenzelektronen, da sie im Periodensystem untereinander stehen. Allerdings sind die Valenzelektronen, dadurch dass das Schwefel-Atom größer ist, besser vom Kern abgeschirmt, weswegen sie sich eher an Reaktionen beteiligen als beim Sauerstoff. Zumindest wurde es eben im Video so erklärt, deshalb glaube ich das jetzt auch mal und das gibt auch Sinn. Deshalb würde ich vermuten, dass (...) das hier (zeigt auf neg. Ladung am S-Atom des 2-Propylthiolats auf S.6) (...) das bessere Nukleophil ist. […] Dass das Schwefel	Emil: It is here [pointing to the S atom of the 2-propanethiolate] that the S minus is more reactive than the O minus. Both have the same number of valence electrons, because they are below each other in the periodic table. However, because the sulfur atom is larger, the valence electrons are better shielded from the nucleus, which is why they participate more in reactions compared to oxygen. At least it was explained in the video in such a way, therefore I know that now - it makes sense to me. Therefore, I would assume that this one [points to 2-propanethiolate] is the better nucleophile. [...] So that sulfur is more likely to attack as a nucleophile, because the electrons are not attracted to the nucleus the way they are with oxygen,

	eher bereit ist zu/ Also dass Schwefel nukleophil eher bereit ist zu reagieren, da die Elektronen nicht so vom Kern angezogen werden, wie es beim Sauerstoff der Fall ist, da dann noch (...) also plump auszudrücken, eine Schicht zwischen ist, die das Ganze abschirmt. Interviewer: Das heißt, du hast dich für das Schwefel-Nukleophil entschieden? Emil: Richtig.	because then there is still … so to put it crudely, there is a layer in-between that shields. Interviewer: You decided to go with the sulfur nucleophile? Emil: Yes. Post-Interview
Results and discussion, Figure 7, p. 2239	Amy: Dadurch, dass das Sauerstoff elektronegativer ist, ähm, greift es die, ähm, partiell positive Ladung vielleicht eher an, weil es noch mehr davon angezogen wird. Weil es noch negativer ist. Weil es die Elektronen vom C noch mehr zu sich zieht. Interviewer: Okay. Wenn es die noch mehr zu sich zieht für die Reaktion. Was macht das für ein Ausschlag Amy: Ja eigentlich würde es halt heißen, dass das schneller geht. Aber / Ja. Ich weiß nicht. Mein Gefühl sagt Schwefel.	Amy: Due to the oxygen being more electronegative, it's [ethanolate] attacking the partial positive charge maybe more because it's attracted to it even more. Because it's even more negative. Because it's [points to oxygen] pulling the electrons from the C even more towards it. Interviewer: “Okay. If it's [oxygen atom] pulling them [the electrons] even more towards it for the reaction, what impact does that have on the reaction? Amy: Yes, actually it would mean that it [points to the reaction with the oxygen nucleophile] goes faster. But / Yes. I don't know. My gut feeling says sulfur. Pre-interview
Results and discussion, Figure 7, p. 2239	Amy: So, das sieht ja sehr ähnlich aus. Und Sauerstoff und Schwefel reagieren eben auch sehr ähnlich, weil sie in der gleichen Gruppe stehen, wobei der Sauerstoff ein bisschen elektronegativer ist. Beim Schwefel ist aber dieser (zeigt auf C-S-Einfachbindung des 2-Propylthiolats) zusätzliche Elektronenzug, sage ich jetzt mal, dadurch, dass eben die hier umliegenden Kohlenstoffatome den mittleren Kohlenstoff quasi ein bisschen von ihrer negativen Ladung abgeben können, das Schwefelatom sich dann noch extra ziehen können und das ist hier halt nicht so stark. Jetzt ist halt die Frage, ja, was ist wichtiger/ Also nicht wichtiger, was ist stärker.	Amy: So, that looks very similar. And oxygen and sulfur also react very similarly because they are in the same group, although oxygen is a bit more electronegative. In the case of sulfur, however, this [pointing to the C-S bond] additional electron pull, I would say, is due to the fact that the surrounding carbon atoms [pointing to the backbone of 2-propanethiolate] can give up a bit of their negative charge to the middle carbon, so to speak, and then the sulfur atom can pull extra, and that is not so strong here [points to ethanolate]. Now the question is, yes, what is more important/ well not more important, [I mean] what is stronger. Post-interview
Results and discussion, Figure 8, p. 2239	Interviewer: Okay. Welche Argumente sprechen für was? Sara: Also die Größe des Moleküls sprechen für mich für das mit dem Sauerstoff und die Ladung eigentlich auch. Aber irgendwie, also mir geht jetzt gerade nicht aus dem Kopf, dass das, was wir in der Studie quasi uns selbst ja beigebracht haben beziehungsweise selber gelernt haben durch die Videos ja auch, das mit der Anzahl der Elektronen und dem Schwefel, dass der Schwefel mehr Elektronen halt hat. Ach, ich weiß auch nicht, ich habe gerade irgendwie eine richtige Blockade irgendwie. Deswegen kann ich damit gerade nicht viel anfangen. Von daher würde ich einfach sagen, das ist das mit dem Sauerstoff das Bessere ist	Interviewer: Okay. What are the arguments in favor of what? Sara: Well, the size of the molecule speaks for me for the one with the oxygen [points to ethanolate] and the charge actually also. But somehow, I can't get it out of my head right now, that what we have taught ourselves in the study or have also learned through the videos, that with the number of electrons…. and the sulfur, that the sulfur has more electrons. Oh, I don't know, I have a real mental block at the moment. That's why I can't do much with it right now. So I would just say that the oxygen is the better one [points to ethanolate]. Interviewer: So you wouldn't know what influence it has if with the electrons… Sara: Well, the difference was that the sulfur can provide its electrons more easily and that they are not so strongly attracted,

	Interviewer: Also du wüsstest nicht, welchen Einfluss es hat, wenn mit den Außenelektronen… Sara: Also der Unterschied war ja quasi, dass der Schwefel seine Elektronen bereitwilliger halt irgendwie zur Verfügung stellen kann und dadurch, dass sie halt nicht so stark angezogen werden, weil die Entfernung ja auch zur positiven Ladung im Schwefel größer ist als beim Sauerstoff. Aber ich kann es irgendwie gerade nicht so in Verbindung bringen mit dem Einfluss auf das Angreifen an dem Kohlenstoff.	because the distance to the positive charge in sulfur is greater than in oxygen. But somehow I can't connect it with the influence on the attack on the carbon. Post-Interview
Results and discussion, Figure 9, p. 2239	Stephen: Ich weiß jetzt nicht, was schneller abläuft. Ich weiß auch nicht, was jetzt von den Endprodukten stabiler wäre und das hier ist ja ein Ether. Und ich glaube, Ether sind relativ stabil und ich denke mal mit Schwefel wird das halt auch stabil sein. Deswegen weiß ich nicht, für was ich mich entscheiden sollte. Interviewer: Was bedeutet stabil…? Stephen: Ja, es zerfällt nicht so schnell. Also da wird jetzt nicht auf einmal die Gruppe, der Alkylrest (zeigt n-Propylrest vom Iso-propyl-n-propylthioether) abfallen oder abgespalten werden, sondern das bleibt dann schon so wie es ist. Interviewer: Um jetzt entscheiden zu können, was schneller läuft, was würde dir da helfen? Stephen: Irgendwelche Kriterien, die einem sagen, was darauf hinweist, was dann schneller abläuft. Ich weiß nicht, wenn es jetzt an der Elektronegativität liegt oder irgendeinem anderen Punkt, der einem dann helfen kann. […] Interviewer: Könntest du dich jetzt hier in dem Moment entscheiden? […] Stephen: Nein, weiß nicht.	Stephen: I don't know now which proceeds faster. I also don't know which of the end products would be more stable and this one is an ether. And I think ethers are relatively stable and I think with sulfur it will be stable. So I don't know what I should choose." Interviewer: What does stable mean to you? Stephen: Yes, it doesn't decompose that quickly. So, the group, the alkyl residue [points to the thioether] will not suddenly fall off or be split off, but it will remain as it is. Interviewer: Now to be able to decide which reaction runs faster, what would help you? Stephen: Any criteria that tells you what indicates what then runs faster. I don't know if it's now because of electronegativity or some other point that can help you then. […]" Interviewer: All right. Could you decide right now here in the moment? Stephen: No, I don't. Pre-Interview
Results and discussion, Figure 9, p. 2239	Also ich denke mal, dass diese Reaktion […]wäre, schneller ablaufen würde, weil das (zeigt auf Ethanolat) meiner Meinung nach ein besseres Nukleophil ist, weil die Ladung dort viel lokalisierter ist als in dem Schwefel (zeigt auf S-Atom des 2-Propylthiolats) oder in dem Molekül halt, zumal der Sauerstoff (zeigt auf neg. geladenes O-Atom des Ethanolats bei neugezeichneter Reaktion) auch eine höhere Elektronegativität hat, eine geringere, aber trotzdem, als S…Das heißt, hier (zeigt auf Ethylrest beim Ethanolat) würden die Elektronen auch noch viel mehr zu dem Sauerstoff (zeigt auf neg. geladenes O-Atom des Ethanolats) gezogen werden als jetzt hier (zeigt auf Kohlenstoffgerüst des 2-Propylthiolats) zu dem Schwefel (zeigt auf S-Atom des 2-Propylthiolats). Deswegen würde das hier (zeigt auf neg. geladenes O-Atom des Ethanolats)	Stephen: So I think that [points to ethanolate] … is in my opinion a better nucleophile, because the charge is much more localized there than in the sulfur [points to S atom of 2-propanethiolate] or in the molecule, especially since the oxygen also has a higher electronegativity….than the sulfur. That means, here [points to ethyl residue of ethanolate] the electrons would also be drawn much more to the oxygen than now here [points to carbon backbone of 2-propanethiolate] to the sulfur. Therefore, this one [points to ethanolate] would be able to react faster than this one [2-propanethiolate]. Post-Interview

	schneller reagieren können als das hier (zeigt auf S-Atom des 2-Propylthiolats).	
Results and discussion, Figure 10, p. 2241	Amy: Dass mit der Aktivierungsenergie war mir, glaube ich, auch nicht so präsent. Also es war mir bewusst irgendwo, das ist ja logisch […] aber das war jetzt nichts worauf ich explizit geachtet hätte, wenn ich mir so eine Reaktion angucke oder zwei Reaktionen vergleiche. Interviewer: Okay. Wenn du jetzt nochmal alle drei Videos in den Kopf rufst, kann du dich dann noch an die Vorgehensweise in den Videos erinnern? Amy: Ja, also ich bin eigentlich/ Beziehungsweise ich bin so vorgegangen, gerade eben, wie in den Videos vorgegangen wurde. Das eben erst die Abgangsgruppe angeschaut wurde, verglichen wurde, dann das Nukleophile, glaube ich, und die Aktivierungsenergie. Also das kann man natürlich nicht einfach so sehen, wenn man eine Reaktion sieht, aber nein, wobei, da war auch der Übergangszustand drin, genau. Genau, dann wurde die Aktivierungsenergie angeguckt und dann war klar, die oder die ist schneller	Amy: I don't think I was that aware of the activation energy either. So I was aware of it at some point, it makes sense to me. …[B]ut that wasn't something I explicitly paid attention to when I looked at a reaction or compared two reactions. Interviewer: Okay. If you now recall all the videos, can you remember the strategy used in the videos? Amy: Yes, so I actually/ Or rather I proceeded in such a way, just now [in the post-interview], as was proceeded in the videos. That first the leaving group was looked at, compared, then the nucleophile, I think, and the activation energy. So you can't just see that [the energy], of course, when you see a reaction….but no, wait, there was also the transition state shown [in the videos], exactly. Exactly, then the activation energy was looked at and then it was clear, this one [reaction] or that one is faster. Post-Interview

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Ein Dank gilt…

allen Mitgliedern der Prüfungskommission

Sehr geehrte Damen und Herren der Prüfungskommission,

ohne die kritische Begutachtung durch Sie wäre der Abschluss meiner Promotion und die Disputation nicht realisierbar. Ich danke Ihnen sehr, dass Sie sich die Zeit nehmen!

allen Proband:innen, die an den Studien teilgenommen haben

Vielen Dank, dass Sie und Ihr Euch die Zeit genommen habt, an unseren Studien teilzunehmen! Die (langen) Interviews haben uns viele Einblicke und Erkenntnisse über Lernprozesse ermöglicht!

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