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Complete List of Authors:	Zaimi, Ina; University of Michigan, Department of Chemistry Dood, Amber; University of Michigan, Department of Chemistry Shultz, Ginger; University of Michigan, Department of Chemistry

ARTICLE

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Ina Zaimi,[a] Amber J. Dood,[a] and Ginger V. Shultz*[a]

Asking students to explain why phenomena occur at a molecular level is vital to increasing their understanding of chemistry concepts. One way to elicit students' mechanistic reasoning and guide construction of knowledge is through Writing-to-Learn (WTL), which is a promising approach for students in organic chemistry courses. In the design of WTL assignments, rhetorical aspects provide an authentic context by designating a role, genre, and audience for students. This context can support students' learning, but, if the rhetorical aspects misalign with the learning objectives of the assignment, they can hinder students' ability to achieve these objectives. In this project, we designed a WTL assignment about a base-free Wittig reaction, which we implemented in an organic chemistry laboratory course. Here, we explore how changes in the rhetorical aspects of this assignment can influence the way students explain two different comparisons of reaction mechanisms. We consider how students use explicit and implicit properties and how the use of these features compares within the context of the reaction. Results indicate that, when the rhetorical aspects align with the learning objectives of the assignment, students provide more productive elaborations that use both explicit and implicit properties. This is supported by both the analysis of students' writing and students' feedback about the assignments.

Introduction

Learning organic chemistry reactions – including but not limited to drawing reaction mechanisms and describing *what* they are as well as explaining *how* and *why* they happen (*i.e.,* reasoning) – is challenging. However, reasoning is broadly a scientific practice (Russ *et al.*, 2008) and specifically a disciplinary practice (Goodwin, 2003). Therefore, an objective of organic chemistry education research is and organic chemistry instruction should be supporting organic chemistry students' reasoning (Dood and Watts, 2023, 2022; Graulich, 2015).

Reasoning in Organic Chemistry

Organic chemistry students can draw reaction mechanisms and describe *what* they represent, although their descriptions tend to be memorized (Dood and Watts, 2023, 2022; Graulich, 2015). Students can also explain *how* they happen, or they can explain *why* they happen (Dood and Watts, 2023, 2022; Graulich, 2015). Explanations that include *how* and *why* reactions happen are part of reasoning about organic reaction mechanisms. Mechanistic reasoning can be broadly defined as an explanation of *how* reactions happen at the electronic level, or at "a lower level" than the observed phenomena does (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015). Instead of describing the molecular transformation, mechanistic reasoning incorporates the electronic transformation with structural entities such as electrons, atoms, and chemical bonds. Mechanistic reasoning can be used in combination with causal reasoning (Dood and Watts, 2023, 2022; Graulich, 2015). Causal reasoning can be broadly defined as an explanation of *why* reactions happen at the molecular level (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015) with explicit properties such as charges and implicit properties such as electrophilicity, nucleophilicity, and leaving group ability. Mechanistic reasoning and causal reasoning can be combined into causal mechanistic reasoning (Dood and Watts, 2023, 2022; Graulich, 2015). Throughout this study, we cite these definitions.

It has been reported in several contexts that students can draw mechanistic arrows and describe how reaction mechanisms happen but not explain the concepts behind the mechanistic arrows (Dood and Watts, 2023, 2022; Graulich, 2015). While students are consistently tasked to draw and describe reaction mechanisms, they are not always required to explain them or provide an underlying reasoning for how and why the reaction mechanisms happen. Research recommends using writing to support students in practicing their mechanistic reasoning and their causal reasoning and, thus, in constructing a deep understanding of organic chemistry reactions (Dood and Watts, 2023, 2022; Finkenstaedt-Quinn *et al.*, 2023).

Researchers have examined a variety of tasks designed to engage students in aspects of reasoning. They designed and studied short-response writing tasks and constructed-response questions (Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood *et al.*, 2020a, 2020b, 2019, 2018; Yik *et al.*, 2021). For example, Cooper *et al.* (2016) designed a writing task on acid-base reactions where students drew

[a] *Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA. E-mail: gshultz@umich.edu*

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the reaction mechanisms and were asked "how" and "why" the reaction mechanisms happen. Cooper *et al.* (2016) determined that students provided more elaborated, more detailed explanations when they asked students the questions separately, rather than jointly. Subsequent research has elicited students' reasoning by using these types of constructed-response questions (Crandell *et al.*, 2020, 2018; Dood *et al.*, 2020a, 2020b, 2019, 2018; Yik *et al.*, 2021).

Additionally, researchers recommended using case-comparison questions (Caspari and Graulich, 2019; Graulich *et al.*, 2019; Graulich and Caspari, 2020; Graulich and Schween, 2018; Rodemer *et al.*, 2020; Watts *et al.*, 2021). For example, Graulich *et. al.* (2019) designed a writing task on substitution reactions where students selected two molecules with similar reactivities out of three molecules. While Graulich *et. al.* (2019) did not analyse for mechanistic explanations and causal explanations, they did analyse for explicit properties and implicit properties, which compose causal explanations. In comparison to students who identified explicit properties, students who identified implicit properties tended to select the correct two molecules (Graulich *et al.*, 2019). Prior and subsequent research has elicited students' reasoning by using these case-comparison questions (Caspari and Graulich, 2019; Graulich and Caspari, 2020; Graulich and Schween, 2018; Rodemer *et al.*, 2020; Watts *et al.*, 2021).

Alternatively, researchers have designed long-response writing assignments, and they have recommended using Writing-to-Learn assignments (Brandfonbrener *et al.*, 2021; Schmidt-Mccormack *et al.*, 2019; Watts *et al.*, 2020). Research has shown that WTL assignments support students' understanding, specifically their understanding of acids and bases (Schmidt-Mccormack *et al.*, 2019), their understanding of nucleophiles and electrophiles (Watts *et al.*, 2020), and their understanding of resonance structures (Brandfonbrener *et al.*, 2021). Moreover, research has suggested that WTL assignments support students' reasoning about reaction mechanisms (Watts *et al.*, 2020). For example, Watts *et al.* (2020) designed a WTL assignment on acid-base reactions where students explained reaction mechanisms. While Watts *et al.* (2020) did not analyse for mechanistic explanations and causal explanations, they did analyse for entities, which compose mechanistic explanations, and properties, which compose causal explanations. All students identified entities, and most students identified properties (Watts *et al.*, 2020). This finding suggests that subsequent research is required to explore how WTL assignments elicit students' reasoning.

Writing-to-Learn Assignments Elicit Student Explanations of Organic Chemistry Reactions

Learning organic chemistry is challenging, and writing supports students' reasoning. However, students may lack motivation because the content may lack relevance (Gilbert, 2006; Stuckey *et al.*, 2013). Increasing relevance by contextualizing the content leads to increasing motivation (Ültay and Çalık, 2012). Studies have shown that "effective" WTL assignments are those that contextualize the content and provide rhetorical aspects (*i.e.,* genre, role, and audience) (Anderson *et al.*, 2015; Bangert-Drowns *et al.*, 2004; Finkenstaedt-Quinn *et al.*, 2023, 2021a; Gere *et al.*, 2019, 2018; Rivard, 1994). Students have perceived these rhetorical aspects to be relevant (Petterson *et al.*, 2021), and, because meaningful learning requires relevance (Bretz, 2001), students have perceived these WTL assignments to be meaningful learning experiences (Gupte *et al.*, 2021). Thus, WTL assignments might motivate students' reasoning, or, minimally, writing more elaborated, more detailed explanations.

Inclusion of rhetorical aspects in a WTL assignment is well documented as a best practice (Anderson *et al.*, 2015; Bangert-Drowns *et al.*, 2004; Finkenstaedt-Quinn *et al.*, 2023, 2021a; Gere *et al.*, 2019, 2018; Rivard, 1994). WTL assignments provide a specified audience because this elicits explanations based on assumptions students hold about the audience (Chen, 2013; Chen *et al.*, 2016; Hand *et al.*, 2004). However, students are still cognizant of the instructor and may address the instructor in their writing as well as the specified audience. For example, Gere *et al.* (2018) found that students' explanations changed if students addressed the audience more than the instructor, the instructor more than the audience, or if the students balanced between audiences. Sometimes, the audience (*e.g.*, a statistical consultant) and the instructor had shared knowledge, and this encouraged students' explanations (Gere *et al.*, 2018). Other times, the audience (*e.g.*, students' grandparents) and the instructor had unshared knowledge, and this constrained students' explanations (Gere *et al.*, 2018). Gupte *et al.* (2021) echoed this finding. These findings suggest that subsequent research is required to explore how WTL assignments' rhetorical aspects shape students' reasoning. Therefore, in response, this study explores not only how a WTL assignment elicits students' reasoning but also how its rhetorical aspects shape students' reasoning.

Succinctly, we designed the Wittig WTL assignment where students explained a traditional intermolecular Wittig reaction mechanism, explained a modified intramolecular Wittig reaction mechanism (Grandane *et al.*, 2019; Schirmer *et al.*, 2015), and compared them. We redesigned the writing assignment, keeping its learning objective but changing its rhetorical aspects. Herein, we explore how students' writing changed when the writing assignment's rhetorical aspects changed.

Theoretical Framework

Flower and Hayes's (1981) "A Cognitive Process Theory of Writing" defines writing cognitively for the writing process and socially for the writing assignment and response.

Cognitively, this theory defines the writing process as a recursive, cyclic process (Figure 1) (Emig, 1977, 1971; Flower and Hayes, 1984, 1981; Hayes and Flower, 1980). First, students plan. Second, students write, or transform internal representations of knowledge (*i.e.*, thinking) into external representations of knowledge (*i.e.*, writing). As delineated by this theory, students' writing captures their thinking, and, specifically, organic chemistry students' writing captures their reasoning, as demonstrated by Watts *et. al.* (2020). Third, students review, which moves them on or moves them into planning and writing. This theory informed the implementation of the Wittig WTL assignment, where students planned and wrote first drafts, provided and received peer reviews, and reviewed and wrote final drafts. Consequently, this theory informed our collection of students' final drafts. Students decided to include – or not to include – concepts from their first drafts to their final drafts in the peer-review process. Watts *et. al.* (2020) asserted that students' final drafts "best captures the features they found important to include."

Figure 1: The Cognitive Process Theory of Writing. A writing response and students' writing process (the dark grey arrows) are in response to a writing assignment and students' motivations (the light grey circle).

Therefore, students' final drafts should capture more complete reasoning than their first drafts would.

Socially, this theory defines a writing assignment as a "rhetorical problem" with its learning objectives and its rhetorical aspects (*i.e.,* genre, audience, and role) and a writing response as a "rhetorical solution" (Figure 1) (Flower and Hayes, 1984, 1981; Hayes and Flower, 1980). Hayes (1996) proposes that students' motivations mediate between the two. Accordingly, students plan, write, and review in response to the writing assignment's learning objectives (*e.g.,* Should I include this concept?), the writing assignment's rhetorical aspects (*e.g.,* Does my audience know this concept? Should I explain this concept?), and their motivations (*e.g.,* Do I want to include this concept? Do I want to explain this concept?). This theory informed our design of the Wittig WTL assignment and our redesigns of its rhetorical aspects, intending to align *problem* and *solution*. Therefore, one assignment's rhetorical aspects should shape more complete reasoning than another assignment's rhetorical aspects would, if the assignment addresses the *problem* or if students' motivation does.

Finally, this theory informed our assessment of the Wittig WTL assignment. We assessed an "effective" assignment as one that *effectively* aligned the *problem*, determined by the assignment's learning objective and rhetorical aspects, and the *solution*, demonstrated by students' final drafts.

Analytical Framework

The Wittig WTL assignment targeted implicit properties (*i.e.* "Students will explain the mechanism's changes by connecting its explicit structures to their implicit properties") because reasoning depends on decoding implicit properties. Considering the assignment's learning objective, we were interested in characterizing one of the first steps in students' reasoning, as Graulich *et al.* (2019) were. We were not interested in characterizing all of the steps in students' reasoning. Thus, we adopted and applied Graulich *et al.*'s (2019) four-code rubric.

Adopting the codes required exemplifying them in regard to the context, the base-free Wittig reaction. Graulich *et al.* (2019) presented two explicit codes: the explicit-descriptive code and the explicit-functional code. We exemplified the explicit-descriptive code, where students stated explicit structures (*e.g.,* an ester group) and explicit properties (*e.g.*, a negative charge) (Table 1). Additionally, we exemplified the explicit-functional code, where students placed explicit structures and explicit properties within a context (*e.g.,* the base-free Wittig reaction) and provided them with a function (*e.g.,* acting as a base) (Table 1).Graulich *et al.* (2019) also presented two implicit codes: the implicit-descriptive code and the implicit-functional code. We exemplified the implicit-descriptive code, where students stated implicit properties (*e.g.,* resonance effects) (Table 1). Additionally, we exemplified the implicit-functional code, where students placed implicit properties within a context (*e.g.,* the base-free Wittig reaction) and provided them with a function (*e.g.,* acting as a base) (Table 1).

Applying the codes required differentiating explicit properties from implicit properties in regard to the content, or the depth of students' statements. Acidity, basicity, and stability are implicit properties, and we found that students could state them as implicit properties. For example, a student stated, *"The acidity is due to the ester group drawing electron density away from the carbon [...]."* Here, acidity was based on the implicit property of induction effects. We read acidity as an implicit property; therefore, we coded the statement as an implicit-descriptive elaboration. However, we found that students could state them as explicit properties. For example, a student stated, *"The [hydrogens] contained in the double bond [of malate] are much more acidic than [the hydrogens] contained in the double bond of acrylate."* Here, acidity was based on the explicit structure of hydrogen, neither based on the explicit property of charge nor based on the implicit properties of pKa, electronegativity, induction effects, or resonance effects. We read acidity as an explicit property; therefore, we coded the statement as an explicit-descriptive elaboration. We had to code the depth of students' statements, although students could have had deeper knowledge and acidity is an implicit property.

Notably, Graulich *et al.* (2019) defined the codes by the depth of students' statements, not by the correctness of them. Implicit statements do support correct statements (Graulich *et al.*, 2019); however, an implicit statement can be either a correct or an incorrect statement, and it is not necessarily more correct than an explicit statement is. Therefore, through our analysis, we captured the elicitation of students' elaborations in contrast to the correctness of their elaborations in order to assess our Wittig WTL assignment.

Research Questions

1. How does the Wittig WTL assignment's rhetorical aspects elicit second-semester organic chemistry students' elaborations?
2. How do second-semester organic chemistry students' elaborations change when the Wittig WTL assignment's rhetorical aspects change?

Table 1: The Codes for the Wittig Writing-to-Learn Responses. The Wittig WTL responses were coded as explicit descriptive (top row), explicit functional (top middle row), implicit descriptive (bottom middle row), and implicit functional (bottom row).

Code	Graulich et al. (2019)'s Definition	Our Definition	Examples
Explicit Descriptive	The student states an explicit property of the molecules.	The student states an explicit structure (*e.g.,* the hydrogen atom, the oxygen atom, the alkene group, the ester group, a resonance structure or a resonance contributor, and a conjugated structure), or the student states an explicit property (*e.g.,* an electron source, an electron sink, the charge of an atom, the symmetry of a group, the acidity of a molecule, the basicity of a molecule, or the stability of a molecule).	*"The starting materials are different by having a ketone [in Scheme 1] and an ester [in Scheme 2]."* *"Acrylate [in Scheme 3] has one CO_2Et, compared to the two [CO_2Ets] that maleate [in Scheme 2] has."*
Explicit Functional	The student states the role of the entity in the problem context, or the student states an explicit property and the problem context.	The student states an explicit structure or an explicit property, and the student provides the explicit structure or the explicit property with a role (*e.g.*, acting as an electrophile, acting as a nucleophile, causing stability, increasing favourability, or increasing likelihood) within the base-free Wittig reaction.	*"[In Scheme 2], an external base is not required, and the deprotonation occurs intramolecularly."* *"[In Scheme 3], this is not possible because the [acrylate] does not have carbon-oxygen double-bonds to push electrons to."*
Implicit Descriptive	The student states an implicit property of the molecules, or the student adds an implicit property to an explicit-functional elaboration.	The student states an implicit property (*e.g.*, the size of an atom, the electronegativity of an atom, the dipole of a bond, the partial charges from the dipole of a bond, the delocalization of electrons in resonance, the conjugation of electrons in resonance, the resonance effects of a group, the induction effects of a group, the electrophilicity of a molecule, the nucleophilicity of a molecule, the acidity of a molecule, the basicity of a molecule, the pKa of a molecule, or the stability of a molecule), or the student adds an implicit property to an explicit-functional elaboration.	*"[In Scheme 2], these features include resonance and the presence of electron withdrawing groups."* *"[In Scheme 3], acrylate does not have this resonance stabilization since it only has one carbonyl group [instead of two carbonyl groups that malate has]."*
Implicit Functional	The student states an implicit property and refers to its role in the problem context.	The student states an implicit property, and the student provides the implicit property with a role (*e.g.,* acting as an electrophile, acting as a nucleophile, causing stability, increasing favourability, or increasing likelihood) within the base-free Wittig reaction.	*"[Maleate's] ester groups stabilize the negative charge by resonance; [the deprotonation] is favourable, however unstable the carbanion is."* *"This is because [...] both esters in maleate are used to stabilize the ylide, [but the] acrylate does not have an additional [ester] group to provide resonance stabilization, so the base-free reaction could not proceed for acrylate."*

Table 2: The Wittig Writing-to-Learn Assignment's Rhetorical Aspects. In 2018, one section was assigned the 2018 Essay – the assignment without rhetorical aspects – and two sections were assigned the 2018 Feature Article – the assignment with rhetorical aspects. In 2021, the three sections choose either the 2021 Medicinal Grant Proposal or the 2021 Ecological Grant Proposal.

Year	Number of Sections (N = 3)	Genre	Role	Audience
2018	1	An Essay for a laboratory course	A student in a laboratory course	An instructor of a laboratory course
	2	A Feature Article for *C&EN*	A reporter for *C&EN*	Readers of *C&EN*
2019	3	A Cover Letter for DowDuPont	An industrial chemist for DowDuPont	Management at DowDuPont
2020	3	A section of a Grant Proposal for NIH	A synthetic chemist in a medicinal research group	Reviewers at NIH
2021	3	A section of a Grant Proposal for NIH	A synthetic chemist in a medicinal research group A synthetic chemist in an ecological research group	Reviewers at NIH

Methods

Our study was situated in a large-enrolment, second-semester organic chemistry laboratory course at the University of Michigan. The course was composed of a four-hour, once-a-week laboratory that was facilitated by graduate teaching assistants (GTAs) and a one-hour, once-a-week lecture that was taught by faculty. The design of this course was guided by the theme of "reasoning," and *reasoning* was defined and implemented in a few requirements. In-lab requirements included lab work, lab reports, case-comparison activities, and quizzes. These case-comparison activities targeted the *reasoning* in multivariable reasoning (Alfieri *et al.*, 2013; Caspari and Graulich, 2019; Graulich and Caspari, 2020; Graulich and Schween, 2018; Watts *et al.*, 2021). Out-of-lab requirements included lab write-ups and WTL assignments (Gupte *et al.*, 2021), recurringly including the Wittig WTL assignment. These lab write-ups targeted the *reasoning* in argumentation (Cruz-Ramí Rez De Arellano and Towns, 2014; Erduran *et al.*, 2004), and these WTL assignments targeted the *reasoning* in casual mechanistic reasoning (Dood and Watts, 2023, 2022; Graulich, 2015). WTL assignments were facilitated and graded by undergraduate teaching assistants (UTAs), or "MWrite Writing Fellows" (Finkenstaedt-Quinn *et al.*, 2021a). Otherwise, assignments were graded by GTAs.

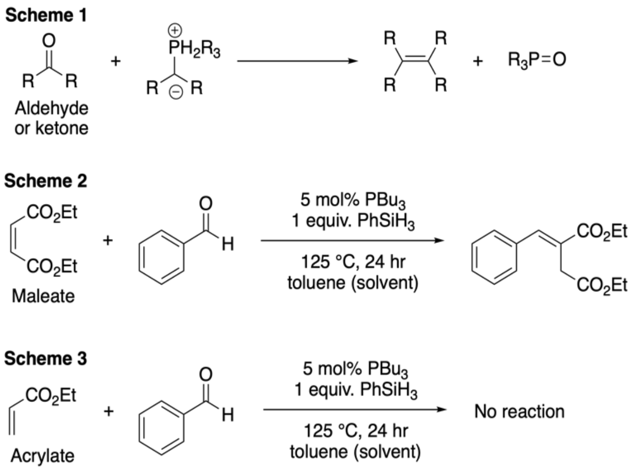

Figure 2: The Wittig Writing-to-Learn Assignment. Scheme 1 was an intermolecular Wittig reaction. Scheme 2 was a successful intramolecular Wittig reaction, but Scheme 3 was an unsuccessful intramolecular Wittig reaction.

Implementing the Wittig Writing-to-Learn Assignment

The assignment spanned two weeks. Using the assignment's directions and questions (Appendix 1), students planned and wrote first drafts in one week. The assignments were submitted onto Canvas, a course management system. Using the peer review's directions and questions (Appendix 2), students reviewed three peers' first drafts and received at least three but at most five peer reviews in three days. The peer review process was a double-blind process that was facilitated by an automated peer review tool (Finkenstaedt-Quinn *et al.*, 2021a) and integrated into Canvas. UTAs assigned first drafts and peer reviews completion-based grades. Using the peer review's directions and questions (Appendix 2) as well as the rubric (Appendix 3), students reviewed their first drafts and wrote final drafts in four days. UTAs assigned final drafts rubric-based grades. After we implemented the assignment, we administered a survey. The surveys were submitted onto Qualtrics, a survey management system. The surveys were optional, so UTAs did not grade them.

Designing the Wittig Writing-to-Learn Assignment

Succinctly, we designed, redesigned, and implemented five assignments. Throughout the implementation, we kept the assignment's learning objective (Figure 2). Scheme 1 was an intermolecular Wittig reaction, but Scheme 2 was an intramolecular Wittig reaction (Grandane *et al.*, 2019; Schirmer *et al.*, 2015). Exploring this, the assignment directed students to propose a reaction mechanism for Scheme 2 (Question 1) and to "compare the mechanistic steps in Scheme 2 to those in Scheme 1" (Question 2) (Appendix 1). The comparison was basicity – either an intermolecular deprotonation or a conjugate addition followed by an intramolecular deprotonation. Moreover, Scheme 2 was a successful intramolecular Wittig reaction, but Scheme 3 was an unsuccessful intramolecular Wittig reaction (Grandane *et al.*, 2019; Schirmer *et al.*, 2015). Exploring this feature, the assignment directed students to "compare the mechanistic steps in Scheme 2 to those in Scheme 3" (Question 3) (Appendix 1). The comparison was acidity – either a stabilized maleate or an unstabilized acrylate. Throughout the implementation, however, we changed the assignment's rhetorical aspects (Table 2). The five assignments were: the 2018 Essay; the 2018 Feature Article; the 2019 Cover Letter; the 2020 Grant Proposal, and the 2021 Grant Proposal.

Specifically, a team of faculty (GVS), postdoctoral scholars (*e.g.,* AJD), graduate research assistants (*e.g.,* IZ), and undergraduate research assistants designed and redsigned five assignments. These changes were based on the Cognitive Process Theory of Writing (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980), the WTL research (Gupte *et al.*, 2021; Petterson *et al.*, 2021), and reflections from research (*i.e.*, the data analysis and our memos) throughout design and from practice (*i.e.,* our conversations with students and UTAs and UTAs' notes) throughout implementation. Yearly, we have considered how vocational interests motivate students (Stuckey *et al.*, 2013) and how students' motivations elicits their responses (Hayes, 1996). For example, in 2020, we discussed relavancy, and we situated the assignment's rhetorical aspects in pre-health students' vocational interests. Therefore, the 2020 Grant Proposal role was a synthetic chemist in a medicinal research group (Table 2). However, Petterson *et al.* (2021) reported that students felt that the assignment's rhetorical aspects, including the Wittig WTL assignment's, were *too* situated in pre-health students' interests. In 2021, we discussed agency, and changed the assignment's rhetorical aspects. Therefore, the 2021 Grant Proposal role was a synthetic chemist in either a medicinal research group or an ecological group. This shifted the focus from instructor-assumed relevancy to student-determined relevancy. We recognize that the assignment's role is a small choice, but we believe that an assignment's design is a series of small choices with a big effect on teaching, learning, and, importantly and specifically, eliciting students' responses.

Designing the Wittig Writing-to-Learn Survey

The survey presented students a series of short-response questions. "What did you find challenging?" and other questions solicited students' feedback on the assignment's design. Contrastingly, "What did you find unclear?" and other questions solicited students' feedback on the assignment's requirements, the assignment's directions, the peer review's directions, and the rubric.

Data Collection

We obtained the Institutional Review Board's approval. We obtained students' consent and anonymized their responses to the assignment and the survey.

We collected final drafts, and, hereafter, "final drafts" and "responses" are synonymous. Although we collected all responses, we found that a random subset of the responses reached saturation. We considered saturation to be when we could present representative, descriptive results but also when we could pull significant conclusions from those results. Therefore, we collected the 2018 Essay responses (n = 100; N = 471), the 2018 Feature Article responses (n = 100, N = 215), the 2019 Cover Letter responses (n = 100; N = 735), the 2020 Grant Proposal responses (n = 100; N = 714), and the 2021 Grant Proposal responses (n = 100; N = 788) via Canvas. We collected the 2018 surveys (N = 147), the 2019 surveys (N = 237), and the 2020 surveys (N = 83) via Qualtrics. No survey was administered in 2021.

Data Analysis

Deductively Coding the Wittig Writing-to-Learn Responses. Two researchers (IZ and AJD) coded the responses (N = 500) via Google Documents. Separately, we coded a subset of the responses (n = 25; N = 500) (κ = 0.8059). Jointly, we adopted the codes, re-coded the subset of the responses, and negotiated consensus (Table 1). Because Cohen's kappa (κ = 0.8059) indicated strong agreement (Cohen, 1960; Watts and Finkenstaedt-Quinn, 2021), one researcher (IZ) coded half of the responses (n = 237; N = 500), and another researcher (AJD) coded half of the responses (n = 238; N = 500).

Our analysis produced two sets of five distributions of four codes. To determine if the distributions of the codes changed when the assignments changed, we conducted a Pearson's chi-square test for homogeneity (McHugh, 2013) via StataSE 17.0. We infrequently applied the explicit-descriptive code, so we removed it, and we only evaluated the explicit-functional, implicit-descriptive, and implicit-functional codes. To determine which distributions of the codes changed, we separated the data by comparison (*i.e.*, the comparison between Scheme 1 and Scheme 2 and the comparison between Scheme 2 and Scheme 3) and conducted Bonferroni pairwise comparisons for each pair of the assignments (Haynes, 2013). We used an adjusted alpha value (α = 0.005) to account for multiple comparisons (Haynes, 2013).

Inductively Coding the Wittig Writing-to-Learn Surveys. Coding the responses emphasized *how* students' elaborations changed, but coding the surveys emphasized *why* students' elaborations changed, with respect to the assignment's rhetorical aspects (*i.e.,* genre, audience, and role). Two researchers (IZ and AJD) coded the surveys (N = 970) via Google Sheets. One researcher (IZ) coded half of the surveys (n = 485; N = 970), and another researcher (AJD) coded half of the surveys (n = 485; N = 970). Separately, we generated codes, capturing these rhetorical aspects. Jointly, we compared and consolidated codes, re-coded all of the surveys, and negotiated consensus. Lastly, we constructed themes, capturing alignment. The Cognitive Process Theory of Writing (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980) posits that the assignment, with its learning objective and its rhetorical aspects, is a "rhetorical

Table 3: The Themes for the Wittig WTL Surveys. The Wittig WTL surveys were sorted as rhetorical aspects misaligning with learning requirements (top row), rhetorical aspects aligning with learning requirements (middle row), or rhetorical aspects engaging students (bottom row).

Theme	Definition	Examples
Rhetorical Aspects Misaligning with Learning Requirements	The assignment's rhetorical aspects misalign with its learning requirements, which hinders students' depth of the elaboration. The students focus on writing the response rather than on explaining the assignment's learning objective.	*"It was unclear – the [audience's] knowledge [...] of organic chemistry. It was stated that they knew some but not all, and it was hard finding that in between point."* *"I [found] it difficult to describe chemistry terminology in a way that is simple but also accurate for the target audience."*
Rhetorical Aspects Aligning with Learning Requirements	The assignment's rhetorical aspects align with its learning requirements, which helps students' depth of the elaboration. The students focus on explaining the assignment's learning objective rather than on writing the response.	*"I liked that [the genre] challenged me to explain this to [the audience] very clearly, but without [...] the technical words that I want to use."* *"It was pretty cool writing a hypothetical grant proposal. [...] I also liked that [the prompt's genre] allowed me to dig deeper about the implications of this reaction."*
Rhetorical Aspects Engaging Students	The assignment's rhetorical aspects engaged the students, which helps students' depth of the elaboration. The students connect the assignment's learning objective to their laboratory course, their lecture course, or their out-of-class experiences.	*"I liked how [the genre] allowed us to put the experiment that we used in the lab into a different situation and perspective."* *"I liked how a lot of the information could be found by reading scientific journals, as [the role] made me practice analysing academic literature."*

problem" but that the response can be a "rhetorical solution." Some students mentioned dissatisfaction in *solving*, so the first theme captured this misalignment between the rhetorical aspects and the learning requirements (Table 3). However, some students mentioned satisfaction in *solving*, so the second theme captured this alignment between the rhetorical aspects and the learning requirements (Table 3). Moreover, some students mentioned engagement in *solving*, and Hayes (1996) proposes that motivation can be a mediator between a *problem* and a *solution*, so the third theme captured this mediation (Table 3).

Limitations

We acknowledge that we were educators, designing and implementing the Wittig WTL assignment, while we were researchers, collecting and analysing students' responses. We rewrote the assignment's rhetorical aspects, and, simultaneously, we revised its questions. These revisions affected the assignment's transparency. We believe transparency builds an equitable learning experience (Winkelmes *et al.*, 2016, 2015); therefore, we were obliged as educators to make these revisions.

An example of these assignment revisions is the 2020 Grant Proposal, which required two pages and recommended that students "write organized and logical paragraphs" and "use clear and concise language." With this assignment, we noticed that the students' responses were longer than the assignment's 2-page requirement, and UTAs repeatedly reported that the students' responses were redundant, neither "organized and logical" nor "clear and concise." We interpreted that the assignment's learning objective (*i.e.,* "Students will explain the mechanism's changes by connecting its explicit structures to their implicit properties") and its questions were misaligned. Thus, students were writing more than they should, oftentimes writing what we wanted them to but sometimes not. In 2021, we pared and revised the questions, where we provided broad directions (*e.g., "*Compare the mechanistic steps in Scheme 2 to those in Scheme 1"), provided specific directions and questions (*e.g.,* "What step allows for the formation of the ylide without the use of an external base?" and "Explain the structural features and electronic, chemical properties that are present or absent in this step"), and defined the vocabulary (*e.g.*, "Structural features are atoms or functional groups") (Appendix 1). Potentially, these transparent questions directed students' responses from superfluous information to explicit and implicit elaborations.

Consequently, these revisions limit our claims. However, we revised how we asked the questions, not the focus of questions themselves or the assignment's learning objective. We found that students' elaborations changed when the assignment's rhetorical aspects changed. Students' surveys and prior research corroborated this influence (Gupte *et al.*, 2021; Petterson *et al.*, 2021). While we cannot claim that the rhetorical aspects were the sole influence, we interpret that the rhetorical aspects were a meaningful influence and that appropriate rhetorical aspects in combination with transparent questions are likely a more meaningful influence.

Additionally, we acknowledge that we implemented this assignment in a single course at a single institution. This implementation affects the assignment's transferability and, consequently, our claims' generalizability. We encourage instructors

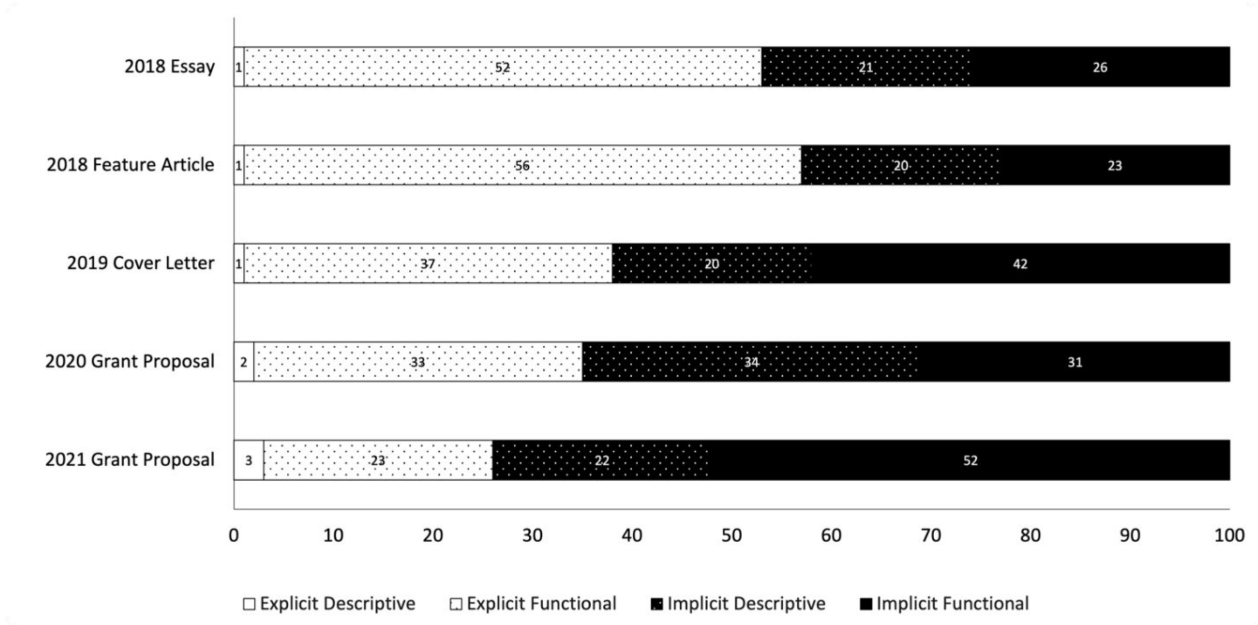

Figure 3: The Distributions of Elaborations for the Comparison between Scheme 1 and Scheme 2. The Wittig WTL responses were coded as explicit descriptive (white bar), explicit functional (white dotted bar), implicit descriptive (black dotted bar), and implicit functional (black bar).

and researchers to implement the 2021 Grant Proposal assignment; however, we encourage them to reflect on the assignment's learning objective, their course's learning objectives, and their institution's context and, accordingly, to alter the assignment.

Results and Discussion

Second-semester organic chemistry students' elaborations changed when the Wittig WTL assignment's rhetorical aspects changed. Addressing the first research question, we discuss the results from the responses, presenting how students' elaborations changed. Addressing the second research question, we discuss the results from the surveys, proposing why students' elaborations changed.

How Students' Elaborations Changed with Changes in the Assignment's Rhetorical Aspects

Students compared a traditional intermolecular Wittig reaction (Scheme 1) to a modified intramolecular Wittig reaction (Scheme 2), in order to connect explicit structures to implicit properties (Figure 2). This comparison was a multivariate comparison, but one of the prime comparisons was the base, which was either a base with a negative charge or the enolate itself with a negatively-charged oxygen and a carbon-carbon double bond. Analysing students' responses, we captured explicit-descriptive, explicit-functional, implicit-descriptive, and implicit-functional elaborations, and Figure 3 presents these elaborations for this first comparison.

As the assignments changed, explicit-functional elaborations decreased and implicit-functional elaborations increased by 2021 (Figure 3). A Pearson's chi-square test ($\chi^2(6) = 41.5$; $p = < 0.001$) confirmed that the assignments had significantly different distributions, and Bonferroni pairwise comparisons (Table 4) found that the 2018 Essay and the 2018 Feature Article had significantly different distributions. Both assignments had more explicit elaborations than implicit elaborations. However, the 2019 Cover Letter, the 2020 Grant Proposal, and the 2021 Grant Proposal had more implicit elaborations than explicit elaborations. Therefore, a cover letter or a grant proposal met the assignment's learning objective more than an essay or a feature article did for the comparison between Scheme 1 and Scheme 2. Exemplifying this finding, we describe one of the first assignments (the 2018 Feature Article) and the final assignment (the 2021 Grant Proposal).

In one of the first assignments (the 2018 Feature Article), students' elaborations were mainly explicit-functional elaborations (Figure 3). Demonstrating explicit-functional elaborations, students stated explicit structures, such as the hydrogen atom, the carbon-

Table 4: Bonferroni Pairwise Comparisons between the Distributions of Elaborations for the Comparison between Scheme 1 and Scheme 2. "2018E" is the 2018 Essay, and "2018FA" is the 2018 Feature Article. *$p \leq 0.005$

Bonferroni Pairwise Comparison	$\chi^2(2)$	*p*
2018E – 2018FA	0.8	0.656
2018E – 2019	19.8	<0.001*
2018E – 2020	9.2	0.01
2018E – 2021	28.5	<0.001*
2018FA – 2019	13.8	0.001*
2018FA – 2020	5.2	0.072
2018FA – 2021	21.1	<0.001*
2019 – 2020	2.4	0.308
2019 – 2021	1.1	0.581
2020 – 2021	6.4	0.040

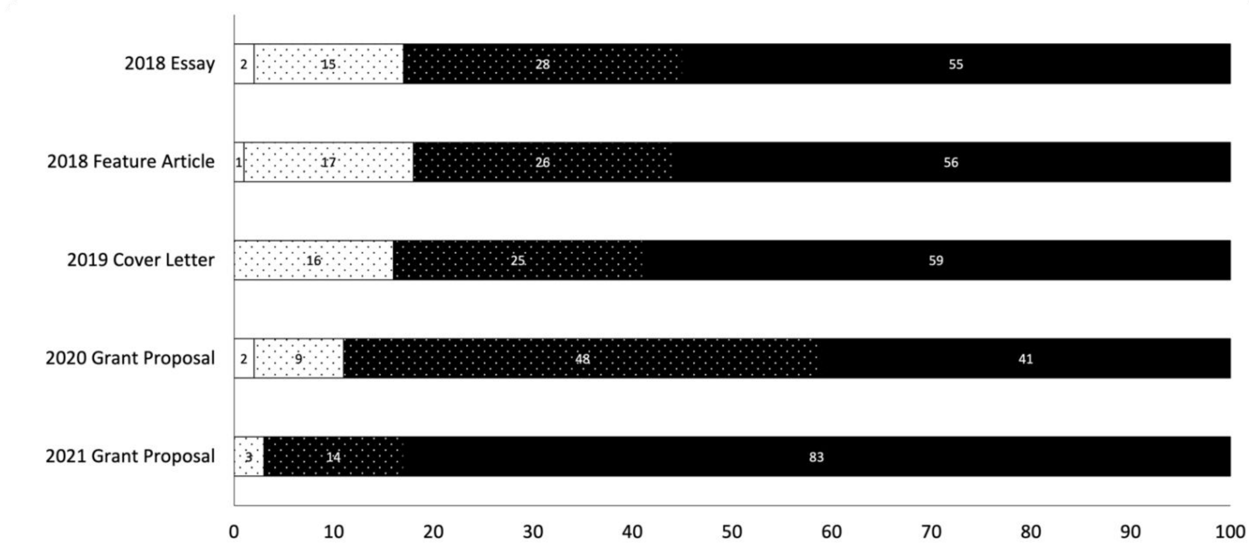

Figure 4: The Distributions of Elaborations for the Comparison between Scheme 2 and Scheme 3. The Wittig WTL responses were coded as explicit descriptive (white bar), explicit functional (white dotted bar), implicit descriptive (black dotted bar), and implicit functional (black bar).

oxygen double bond, or the carbon-carbon double bond. For example, a student connected having a hydrogen atom to being an acid, "*This hydrogen is acidic due to the carbonyl group […].*" Acidity was based on the hydrogen atom and the ester group, pulling on explicit structures. Also demonstrating explicit-functional elaborations, students stated explicit properties, such as the negatively-charged oxygen, the negatively-charged carbon, or the positively-charged phosphorus. For example, a different student connected having a negatively-charged carbon to being a base,

> *"The electrons on the O slide down, and the C-C double bond deprotonates the acidic H attached to the C with the P group […]. [Those] electrons fall into a C-P double bond […]. [In the] traditional mechanism, a separate base deprotonates […]. In this mechanism, the deprotonation occurs intramolecularly – hence why no base is needed."*

Basicity was based on the negatively-charged oxygen or the negatively-charged carbon, pulling on explicit properties. This focus on decoding explicit structures and explicit properties is a focus on explaining *how* the step happens, with explicit structures (*e.g., "a base deprotonates"*) and explicit properties (*e.g., "the electrons slide down"*) being actors in the step. Thus, these elaborations can be read as students practicing their mechanistic reasoning (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015).

Contrastingly, in the last assignment (the 2021 Grant Proposal), students' elaborations were mainly implicit-functional elaborations (Figure 3). Demonstrating implicit-functional elaborations, students stated implicit properties, such as induction effects or resonance effects. For example, a student connected having induction effects to being an acid,

> *"The structural differences [between] the base-free Wittig reaction [and] the Wittig reaction are the carbonyl groups and the alkene. [These] double bonds provide electron shifting […]. [...] Specifically, the hydrogen is acidic – or is easier to deprotonate – because the carbonyl groups withdraw electron density from the [neutral] carbon… "*

Acidity was based not only on the hydrogen atom and the ester group but also on induction effects, pulling on an implicit property. The same student continued and connected having resonance effects to being a base,

> *"...and because the negatively-charged carbon [will be] resonance-stabilized by the carbonyl groups […]. [Resonance and induction] confer the deprotonation by the alkene and the elimination of a strong, external base."*

Basicity was based on not only the negatively-charged carbon and the negatively-charged carbon but also on resonance effects, pulling on an implicit property. This focus on decoding implicit properties is a focus on explaining *why* the step happens, with implicit properties (*e.g., "easier to deprotonate"*) being descriptors of the step. Thus, these elaborations can be read as students practicing their causal reasoning (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015).

Additionally, students compared a successful intramolecular Wittig reaction (Scheme 2) to an unsuccessful Wittig reaction (Scheme 3), in order to connect explicit structures to implicit properties (Figure 2). This comparison was a univariate comparison, and the prime comparison was the acid, either the maleate with two ester groups or the acrylate with one ester group. Analysing students' responses, we captured explicit-descriptive, explicit-functional, implicit-descriptive, and implicit-functional elaborations, and Figure 4 presents these elaborations for this second comparison.

As the assignments changed, implicit-functional elaborations stayed constant from 2018 to 2020, but they increased by 2021 (Figure 4). A Pearson's chi-square test ($\chi 2(6) = 31.5$; $p = <0.001$) confirmed that the assignments had significantly different distributions, and Bonferroni pairwise comparisons (Table 5) found that the 2021 Grant Proposal had the significantly different distribution. The 2021 Grant Proposal had the most implicit elaborations, although all assignments had more implicit

Table 5: Bonferroni Pairwise Comparisons between the Distributions of Elaborations for the Comparison between Scheme 2 and Scheme 3. "2018E" is the 2018 Essay, and "2018FA" is the 2018 Feature Article. *$p \leq 0.005$

Bonferroni Pairwise Comparison	$\chi^2(2)$	*p*
2018E – 2018FA	0.1	0.958
2018E – 2019	2.0	0.366
2018E – 2020	0.5	0.767
2018E – 2021	23.8	<0.001*
2018FA – 2019	1.3	0.521
2018FA – 2020	0.8	0.678
2018FA – 2021	22.0	<0.001*
2019 – 2020	3.7	0.156
2019 – 2021	18.5	<0.001*
2020 – 2021	22.3	<0.001*

elaborations than explicit elaborations. Therefore, an essay, a feature article, a cover letter, or a grant proposal meets the assignment's objective for the comparison between Scheme 2 and Scheme 3. Exemplifying this finding, we describe the last assignment (the 2021 Grant Proposal).

In the last assignment (the 2021 Grant Proposal), students' elaborations were mainly implicit-functional elaborations (Figure 4). Demonstrating implicit-functional elaborations, students stated implicit properties, such as induction effects or resonance effects. For example, a student connected having induction effects to being an acid,

> "*[Scheme 3] lacks a second electron-withdrawing carbonyl group [...]. [...] The C-H bond in acrylate is stronger than the C-H bond in maleate [since] acrylate lacks the electron-withdrawing carbonyl that inductively weakens [maleate's] C-H bond. [This] makes [acrylate's] H less acidic, [and], if deprotonated, the structure would lack resonance stabilization. As this H cannot be intramolecularly deprotonated and no other bases [are] present, the acrylate cannot be turned into a ylide."*

Acidity was based on: the ester group, starting with an explicit structure; induction effects, continuing with an implicit property; and bond strength, ending with another implicit property. Like the implicit-functional elaborations in the first comparison, these elaborations focus on decoding implicit properties (*e.g., "is stronger"*), focus on explaining *why* the step happens, and can be read as students practicing their causal reasoning (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015). Unlike the implicit-functional elaborations in the first comparison, these elaborations start with an explicit structure, connect the explicit structure to an implicit property, and continue with a series of implicit properties or "chain" (Graulich *et al.*, 2019) (*e.g., "acrylate lacks the electron-withdrawing carbonyl that inductively weakens [maleate's] C-H bond"*) and can be read as students practicing more chained, more elaborated causal reasoning.

Both comparisons are engaging students in decoding implicit properties; thus, both comparisons are engaging students in causal reasoning (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015). However, the second comparison is engaging students in chaining implicit properties, or in more chained, more elaborated causal reasoning. This difference in the depth could be due to the difference in the comparison. The second comparison is a univariate comparison, where students decoded one explicit structure and constructed an elaboration from this explicit structure to multiple implicit properties. Contrastingly, the first comparison is a multivariate comparison, where students decoded multiple explicit structures and they constructed an elaboration from one of these explicit structures to one implicit property. Presumably, students weighed these explicit structures, after they decoded them and before they explained one of them. Accordingly, these elaborations are engaging students in multivariate reasoning (Bodé *et al.*, 2019; Deng and Flynn, 2020; Kraft *et al.*, 2010; Moreira *et al.*, 2019; Sevian and Talanquer, 2014; Strickland *et al.*, 2010; Weinrich and Talanquer, 2016), in addition to their causal reasoning (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015). Engaging in both may be limiting the depth. Research has shown that a case comparison elicits multivariate reasoning (Caspari *et al.*, 2018; Caspari and Graulich, 2019; Graulich and Caspari, 2020; Watts *et al.*, 2021). Consequently, we assume that students' multivariate reasoning is shaped by the question's case comparison, but we conjecture that their causal reasoning may be shaped by the assignment's rhetorical aspects.

Why Elaborations Changed According to How Students Perceived the Assignment's Rhetorical Aspects

Students responded to surveys and commented on the assignment, including but not limited to the assignment's rhetorical aspects and its learning requirements. Analysing students' comments and guided by the Cognitive Process Theory of Writing (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980), we constructed three themes: rhetorical aspects misaligning with learning requirements; rhetorical aspects aligning with learning requirements; and rhetorical aspects engaging students (Table 3). This theory posits that the assignment, with its learning objective and its rhetorical aspects, is a "rhetorical problem" but that the response can be a "rhetorical solution." Exemplifying our themes, we describe one of the first assignments (the Feature Article) and one of the final assignments (the Grant Proposal).

In one of the first assignments (the Feature Article), students' comments suggested that the rhetorical aspects and the learning requirements were misaligned. Defining this theme, the specified audience frustrated students. Specifically, a student felt frustrated interpreting *C&EN* readers' knowledge, *"It was unclear – the [audience's] knowledge [...] of organic chemistry. It was stated that they knew some but not all, and it was hard finding that in between point."* This student interpreted that readers have some knowledge. Similarly, a student felt frustrated translating *C&EN* readers' knowledge, *"The translation of organic chemistry was unclear. How was I supposed to talk about [organic chemistry to] someone who doesn't know a lot about [organic chemistry]?"* This student interpreted that *C&EN* readers do not have any knowledge. Students interpreted that *C&EN* readers are not a scientific audience, without any or with some knowledge, although we intended that they would be a general scientific audience.

Also defining this theme, the specified audience appeared to constrain students' elaborations. Specifically, a student focused on formatting the response, "*[The audience] was counterproductive and caused me to spend more time worrying about the formatting and writing style of the assignment instead of the content.*" Similarly, a student focused on simplifying the response, *"I [found] it difficult to describe chemistry terminology in a way that is simple but also accurate for the target audience."* Both students focused on writing the response, including style and length, rather than explaining the assignment's objective. Because students interpreted that *C&EN* readers are not a scientific audience, they assumed that vocabulary, phrases, and concepts were not shared and should be explained. However, the explanation must be *"simplified"* and explicit but also elaborated and implicit. Therefore, the audience poses an unsolvable *rhetorical problem*, choosing either fulfilling the assignment's rhetorical aspects or explaining the assignment's learning objective. This could account for the 2018 Feature Article not meeting the assignment's learning objective.

Contrastingly, in one of the final assignments (the Grant Proposal), students' comments suggested that the rhetorical aspects and the learning requirements were aligned. Defining this theme, the audience satisfied students. For example, a student felt satisfied translating NIH readers' knowledge, *"I liked that [the genre] challenged me to explain this to [the audience] very clearly, but without [...] the technical words that I want to use."* This student interpreted that reviewers have most knowledge. Students interpreted that NIH readers are a scientific audience, without all but with most knowledge, and we intended that they would be a specific scientific audience.

Also defining this theme, the specified audience appeared to encourage students' elaborations. For example, a student focused on *"working out"* the reaction mechanisms, *"...[I]t is a fun challenge to write a highly technical essay. Working out the mechanism is very rewarding, as I feel like I have done something really difficult well."* This student focused on explaining the assignment's objective rather than on writing the response, including style and length. If students focused on writing the response, they focused on the length because they wanted to write more, not because they could not write more or did not know how much to write. For example, a student felt frustrated keeping to an assigned length, *"A challenging part of the assignment was [...] keeping my word [count] to a minimum."* Because students interpreted that NIH readers are a scientific audience, they assumed that most vocabulary, phrases, and concepts were shared and that the salient ones should be explained. Moreover, the explanation could be elaborated and implicit. Therefore, the audience poses a solvable *rhetorical problem*, balancing the assignment's rhetorical aspects and explaining the assignment's learning objective. This could account for the 2020 and 2021 Grant Proposals meeting the assignment's learning objective.

These findings show the influence of specifying an appropriate audience. We conjecture that students' elaborations may be shaped by the assignment's audience, but we recognize that their elaborations may be truly shaped by their interpretations of the assignment's audience. Therefore, WTL assignments should not only specify an audience (Gere *et al.*, 2019) but also detail an appropriate, transparent audience and describe the audience's level of knowledge or provide examples.

Additionally, we recognize that students' elaborations may be shaped by their motivations. The Cognitive Process Theory of Writing (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980) proposes that students not only write in response to the assignment's learning objectives (*e.g.,* Should I include this concept?) and its rhetorical aspects (*e.g.,* Does my audience know this concept? Should I explain this concept?) but also in response to their motivations (*e.g.,* Do I want to include this concept? Do I want to explain this concept?). Students' comments suggested that they were engaged. Defining this theme, students commented that the assignment *"motivated [them],"* the assignment *"seemed meaningful,"* or the assignment *"seemed relevant."* Expanding on the assignment's relevance, a student connected the 2018 Feature Article to their laboratory course, *"I like how [the assignment] incorporated what we were doing in the lab."* Similarly expanding on the assignment's relevance, a student connected the 2020 Grant Proposal to their lecture course, *"I like that this assignment built upon [what] we had covered in lecture. The material was not totally unfamiliar, so I could actually attempt to explain it on my own."* Students found this assignment to be relevant, and studies corroborate that students find our assignments to be relevant (Petterson *et al.*, 2021) and, because meaningful learning requires relevance (Bretz, 2001), that they find them to be meaningful learning experiences (Gupte *et al.*, 2021). Relatedly, because motivation requires relevance (Stuckey *et al.*, 2013), students might find our assignments to be motivating experiences. These findings inform ours, as students' motivations have been proposed to mediate between an assignment's *rhetorical problem* (*e.g.,* the audience) and its *rhetorical solution* (Hayes, 1996). Thus, we suspect that appropriate rhetorical aspects are those that motivate students in addition to – or in order to – encourage their elaborations.

Conclusion and Implications

WTL assignments support a variety of learning objectives, including those specific to organic chemistry (Brandfonbrener *et al.*, 2021; Schmidt-Mccormack *et al.*, 2019; Watts *et al.*, 2020). Expanding these learning objectives, we iteratively designed a WTL assignment that targeted implicit properties (*i.e.,* "Students will explain the mechanism's changes by connecting its explicit structures to their implicit properties"). We implemented five assignments. Previous research demonstrated that implementing WTL assignments does not guarantee students' learning will be supported (Anderson *et al.*, 2015; Applebee, 1984; Bangert-Drowns *et al.*, 2004; Finkenstaedt-Quinn *et al.*, 2023, 2021a; Gere *et al.*, 2019; Rivard, 1994). Specifying rhetorical aspects is identified as important in supporting students' learning, but different assignments, depending on their genre, audience, and role, have different learning outcomes (Chen, 2013; Chen *et al.*, 2016; Gere *et al.*, 2018; Hand *et al.*, 2004). Therefore, we not only explored how the assignment elicited students' writing but also how students' writing changed when the assignment's rhetorical aspects changed.

The assignments elicited students' explicit and implicit elaborations. Mechanistic reasoning depends on explicit elaborations, or decoding explicit structures (*e.g.,* electrons, atoms, and chemical bonds); similarly, causal reasoning depends on implicit elaborations, or decoding implicit properties (*e.g.,* acidity, induction effects, or resonance effects) (Bodé *et al.*, 2019; Cooper *et al.*, 2016; Crandell *et al.*, 2020, 2018; Dood and Watts, 2022; Russ *et al.*, 2008; Yan and Talanquer, 2015). Thus, these elaborations can be interpreted as students practicing their reasoning and demonstrating their reasoning to researchers or instructors. The 2018 Essay and the 2018 Feature Article did not elicit these implicit elaborations to the extent that the 2019 Cover Letter, the 2020 Grant Proposal, and the 2021 Grant Proposal did, and, thus, the latter assignments better met the learning objective. Consistent with Watts et al.'s (2020) findings, our findings suggest that WTL assignments can support the learning objective of reasoning, in addition to the learning objectives of conceptual understanding that have been documented previously (Brandfonbrener *et al.*, 2021; Finkenstaedt-Quinn *et al.*, 2023; Schmidt-Mccormack *et al.*, 2019; Watts *et al.*, 2020).

Moreover, the assignments shaped students' elaborations, moving from explicit elaborations to implicit elaborations. According to Flower and Hayes, the writing assignment is the "rhetorical problem," and the writing response is the "rhetorical solution" (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980) and an assignment's rhetorical aspects are one of the mediators between *problem* and *solution* (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980). The 2018 Feature Article constrained students' elaborations into explicit elaborations. Contextualizing this finding, students' comments expressed that this assignment's audience presented a challenging and disengaging *problem*. Students interpreted that *C&EN* readers are not a scientific audience, although we intended that they would be a general scientific audience. They reported feeling frustrated, focusing on writing the response. Thus, the assignments' rhetorical aspects and learning requirements were misaligned. Contrastingly, the 2020 and 2021 Grant Proposal assignments encouraged their elaborations into implicit elaborations. Contextualizing this finding, students' comments expressed that this assignment's audience presented a challenging but engaging *problem*. We intended that NIH reviewers would be a specific scientific audience, and students interpreted that they were. They reported feeling satisfied and capable, focusing on explaining the assignment's learning objective. Therefore, the assignments' rhetorical aspects and learning requirements were aligned. These findings show how WTL assignments need to detail *appropriate* rhetorical aspects in order to encourage more implicit elaborations and, correspondingly, more complex reasoning.

Students' motivations are also one of the mediators between *problem* and *solution* (Flower and Hayes, 1984, 1981; Hayes, 1996; Hayes and Flower, 1980). Students' comments expressed that all assignments "motivated them," "seemed relevant," and "seemed meaningful." Studies corroborate that students find WTL assignments to be relevant (Petterson *et al.*, 2021) and to be meaningful learning experiences (Gupte *et al.*, 2021). Supporting these findings, we report how WTL assignments need *relevant* rhetorical aspects in order to encourage more implicit elaborations and, correspondingly, more complex reasoning.

Implications for Research

Our findings support previous reports that WTL assignments can elicit organic chemistry students' reasoning on reaction mechanisms. Researchers can transform our writing assignment into a writing task, interview questions, or survey questions, aiding them in eliciting students' reasoning. However, we designed this assignment on a single case (*i.e.*, the Wittig reaction), and we implemented this assignment in a single course at a single institution. We encourage designing writing assignments on other reaction cases and implementing them in different contexts.

Implications for Instruction

Organic chemistry instructors can implement our writing assignment, aiding them in assessing students' reasoning. However, we recommend adapting the assignment, especially setting learning objectives for a type of reasoning or parts of reasoning, detailing appropriate and relevant rhetorical aspects, and aligning the learning objectives and the rhetorical aspects. These rhetorical aspects can be inspired by historical moments (*e.g,* synthesizing aspirin or thalidomide), scientific aspirations (*e.g.,* writing a grant proposal) and vocational interests (*e.g.,* a synthetic chemist in a medicinal research group), or students themselves (*e.g.,* What organic molecule is important to you?). We suggest Finkenstaedt-Quinn *et al*. (2021a) and Finkenstaedt-Quinn *et al*. (2023) for guidance on designing and implementing WTL assignments in STEM courses as well as Finkenstaedt-Quinn *et al*. (2021b) for guidance on peer review in all courses and, possibly, peer assessment in courses without UTAs or GTAs.

Author Contributions

All authors contributed. IZ and AJD contributed to the conceptualization, the data collection, analysis, and presentation, and the writing of this study. GVS contributed to the design and implementation of the assignment as well as the revising of this study. The manuscript was written by IZ, with extensive, valuable feedback from AJD and GVS. All authors read and approved the manuscript.

Conflicts of Interest

There are no conflicts to declare.

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Appendix 1: The 2021 Grant Proposal Assignment

Motivation and Significance

Benzoxepine (Figure 5) is a heterocycle composed of a six-membered benzene ring and a seven-membered oxepin ring. Some benzoxepine analogs inhibit tuberculosis, and other benzoxepine analogs inhibit cancers by inducing activation of the apoptosis pathway. Specifically, **benzoxepinoisoxazolone** (Figure 6) is a benzoxepine analog whose anticancer activity is attributed to its functionalization with phenyl and azole groups.

Benzoxepine analogs are important intermediates in the synthesis of therapeutic drugs. However, the isolation of benzoxepine analogs from natural sources is inefficient. Recently, German researchers synthesized benzoxepine analogs (Figure 7) using a **base-free Wittig reaction** (Figure 8). This reaction allows for the synthesis of therapeutic drugs on an industrial scale.

Application

You are a medicinal drug developer in a research group that primarily studies anticancer compounds. Inspired by the benzoxepinoisoxazolone in Figure 2, one of the group's current goals is synthesizing benzoxepine analogs using the base-free Wittig synthesis and evaluating the analogs for anticancer activities. To do so, your project team is drafting a grant proposal for the National Institute of Health (NIH) that summarizes the project's goals and argues for the project's significance, innovation, and impact. **You, the organic chemist expert, must write the section of the grant proposal that explains the base-free Wittig reaction.** Because the reaction is critical for the success of the project, you must demonstrate to the committee that your project team understands how the reaction works and why it is selective. The committee who will review the proposal is made up of scientists from many disciplines, including chemistry, biology, and medicine. Therefore, they may not be experts when it concerns mechanisms or organic-specific terms. The NIH recommends that you:

- write organized and logical paragraphs with headers;
- include figures that assist the reviewers in understanding complex information;
- use clear and concise language, striking a balance between organic jargon and oversimplifications.

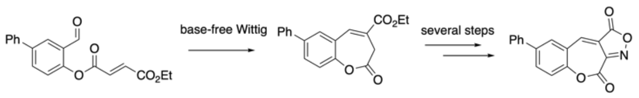

Figure 5: Synthesis of benzoxepinoisoxazolone using the base-free Wittig reaction.

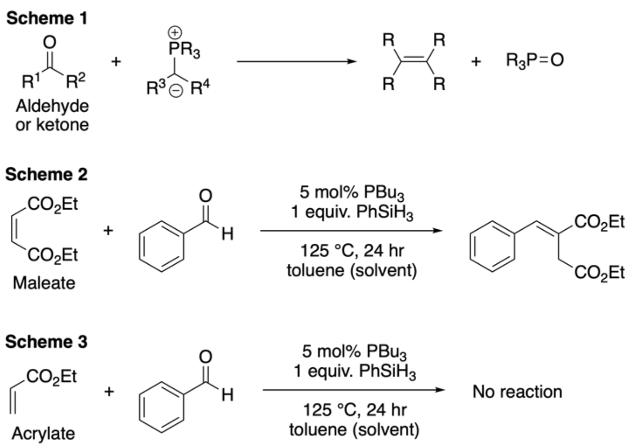

Figure 6: Generalized schemes of the base-free Wittig reaction. Scheme 1 shows the standard Wittig reaction, and Scheme 2 shows an example of the base-free Wittig reaction using a maleate starting material. Scheme 3 shows a limitation of the base-free Wittig, where the reaction fails when using an acrylate starting material.

Requirements

Your section of the grant proposal should be approximately between 500-700 words (1-2 pages) in length. It should address the following points:

1. What changes occur from the starting materials and the reagents to the products for the reaction in Scheme 2?
   a. Describe the mechanistic steps.
   b. Explain the structural features (*e.g.,* atoms or functional groups) and the electronic, chemical properties (*e.g.,* electronegativity, resonance, or induction) of the starting materials, reagents, and intermediates, and, moreover, explain their role (*e.g.,* electrophile, nucleophile, acid, or base) or arrows in the mechanistic step.
   c. Focus on the *how* and *why* as well as the *what.*
2. Compare the mechanistic steps in Scheme 2 to those in Scheme 1.
   a. What step allows for the formation of the ylide without the use of an external base? (Note that the ylide is not shown in this scheme.)
   b. Explain the structural features and electronic, chemical properties that are present or absent in this step.
3. Compare the mechanistic steps in Scheme 2 to those in Scheme 3.
   a. Why does the reaction work with maleate but not work with acrylate?
   b. Explain the structural features and electronic, chemical properties that are present or absent in this step.

You can and should include figures of schemes, structures, or mechanisms, if that supports your response. We suggest that you have the figure(s) in front of you — ready to color-code or mark-up in various ways — and that you use your visible thinking to guide your audience through your writing. Any images that you include in your response, including the figures in this prompt or those that you draw in ChemDraw or on paper, must have the original source cited using either ACS or APA format. **Given your audience, your written response should suffice so that the written response is as representative and descriptive as the figures. You will be graded only on your written response.**

Appendix 2: The 2021 Peer Review

Directions

- Print and read over your peer's response to quickly get an overview of the piece.
- Read the response more slowly, keeping the rubric in mind.
- Highlight the pieces of text that let you directly address the rubric in your online responses.
- In your online responses, focus on higher-order concerns, like content and argument, rather than lower-order concerns, like grammar and spelling.
- Be very specific in your responses, referring to your peer's actual language, mentioning terms and concepts that are either present or missing, and following the directions in the rubric.
- Use respectful language, whether you are suggesting improvements to or praising your peer.

Questions

1. Does the author describe and explain the mechanistic steps in Scheme 2 so that the committee can easily, swiftly understand how the reaction works? Comment on the parts of the response where the author could improve their mechanistic descriptions of *what* electronic movement occurs as well as their mechanistic explanations of *how* and *why* electronic movement occurs.
2. Does the author's comparison provide a description (the *what*) as well as an explanation (the *how* and *why*) of Scheme 1 occurring intermolecularly but Scheme 2 occurring intramolecularly? Comment on the structure and the electronic, chemical property that the author attributes as the reason.
3. Does the author's comparison provide a description as well as an explanation of Scheme 2 occurring but Scheme 3 not occurring? Comment on the structure and the electronic, chemical property that the author attributes as the reason.

Appendix 3: The 2021 Grant Proposal Rubric

Criteria	"Attempts" This Criterion	Points (___ / 25)
Description and Explanation of Scheme 2	Includes: • A CORRECT description of the structural features OR *what* changes happen in the reaction mechanism AND • A CORRECT explanation of the electronic, chemical properties OR *how* and *why* changes happen in the reaction mechanism	10
Comparison of Scheme 1 and Scheme 2	Provides: • A structural feature as the comparison OR • A structural feature and its electronic, chemical property as the comparison *Criterion (2) may be repetitive of Criterion (1), but Criterion (2) adds onto Criterion (1)'s explanation with a direct comparison between Schemes 1 and 2*	3
Comparison of Scheme 2 and Scheme 3	Includes: • A CORRECT description of the structural features OR *what* changes happen in the reaction mechanism AND • A CORRECT explanation of the electronic, chemical properties OR *how* and *why* changes happen in the reaction mechanism	10
Appropriate Language	Attempts: • Clear, concise sentences and logical, organized paragraphs *DO NOT omit the point if they do not adhere to the grant proposal style*	1
Citations	Attempts: • Citations for figures they did not produce • Indications for figures they did produce (either ChemDraw or hand-drawn)	1