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Utility of creative exercises as an assessment tool for revealing student conceptions in organic chemistry

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Creative exercises (CEs) consist of open-ended prompts to which students provide a series of relevant, distinct, and accurate statements, thus requiring that students make connections between concepts. In this study, CEs were incorporated into a one-semester *Survey of Organic Chemistry* course to identify what connections between chemistry concepts students made and what incorrect conceptions or misconceptions about chemistry students held. Students ($N = 79$) enrolled in the course first completed a practice CE as an in-class group activity followed by individually responding to a CE bonus problem on each of their four course exams. The number of different concepts students addressed for each CE increased over the semester, indicating that students made increasing content connections about course material; however, misconceptions about early concepts, such as nomenclature and assigning configurations, remained consistent throughout the semester. Furthermore, the CEs were found to be instrumental in shedding light on misconceptions and knowledge structures of students across varying performance levels. Overall, students reported that they viewed the CEs favorably and would like to see CEs incorporated in future courses.

Introduction

Organic chemistry is often considered a “weed-out” course, with some universities’ reported attrition rates as high as 30-50% (Grove *et al.*, 2008; Grove and Bretz, 2012). Unfortunately, many students struggle to understand the material which results in students failing or withdrawing from the course. This difficulty often arises because students rely on rote memorization of individual reactions rather than learning how each of the concepts connect and work together as part of a bigger whole (Grove and Bretz, 2012; Anzovino and Bretz, 2016).

Instead of rote memorization, organic chemistry requires that students forge connections among diverse chemistry concepts to perform tasks such as interpreting chemical representations, proposing mechanisms, and making structure–reactivity judgments (Graulich, 2015). This process of actively interlinking concepts and developing schemas fosters meaningful learning, which is crucial for students to be able to apply their knowledge to novel situations. Given the superiority of meaningful learning over rote memorization, a variety of instructional approaches for cultivating meaningful learning in organic chemistry have been reported, including writing-to-learn activities (Gupte *et al.*, 2021), using a flipped organic chemistry classroom (Fautch, 2015; Flynn, 2015), incorporating “Bridge activities” in flipped classrooms (Stewart and Dake, 2019), and completely transforming the organic chemistry curriculum (Grove and Bretz, 2012; Cooper *et al.*, 2019). In turn, reliable assessments capable of measuring meaningful student learning and connection-making within organic chemistry must be developed and evaluated. Two types of assessments already reported in the literature for measuring student connection-making include concept maps (CMs) and creative exercises (CEs).

CMs have garnered widespread use in chemistry courses due to their capacity to facilitate the integration of ideas. CMs, originally developed by Novak in 1972 (Novak and Cañas, 2006), are visual tools that use a series of nodes and links to summarize, organize, and represent meaningful relationships between concepts (Wong *et al.*, 2021). CMs have been found to enhance student learning, and thus instructors have been encouraged to incorporate CMs into the curriculum (Nesbit and Adesope, 2016; Schroeder *et al.*, 2018). Within organic chemistry, CMs have found utility as both a teaching tool (Šket *et al.*, 2015) and an assessment tool (Lopez *et al.*, 2011; Vachliotis *et al.*, 2014; Burrows and Mooring, 2015; Anzovino and Bretz, 2016).

However, due to their open-ended and individualistic nature, a key limitation of CMs arises from the difficulty to ensure consistent scoring. In fact, a study by Johnstone and Otis (2006) revealed that student-generated CMs exhibited only a weak correlation with proficient students’ course content understanding. This discrepancy arose because the students with a proficient understanding utilized CMs as keys to access their broader knowledge base rather than as accurate representations

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3 of their content comprehension. Consequently, CMs have been recognized as valuable primarily for formative assessments in
4 college-level chemistry courses (Schwendimann, 2015; Gilewski *et al.*, 2019).

5 In contrast to CMs, CEs, which were originally developed by Trigwell and Sleet (1990), offer distinct advantages because
6 they are simpler to grade, rendering them suitable for both formative and summative assessments in college-level chemistry
7 courses (Ye and Lewis, 2014; Gilewski *et al.*, 2019). CEs consist of a prompt to which students provide a list of relevant, distinct,
8 and accurate statements. The instructor sets a minimum number of correct statements necessary to receive full credit, typically
9 ranging from one-third to one-half of those identified by the instructor (Ye and Lewis, 2014). A key advantage of CEs is their
10 capacity to enable instructors to discern not only what students comprehend, but also to identify any misconceptions or
11 inappropriate conceptions students may hold (Lewis *et al.*, 2010). In addition, like CMs, CEs have also been shown to promote
12 connection-making among concepts in chemistry (Ye and Lewis, 2014; Gilewski *et al.*, 2019; Ye *et al.*, 2020).

13 CEs have been utilized across various chemistry courses, showcasing their versatility and effectiveness. For
14 instance, in the realm of general chemistry, there is a wide literature base addressing CEs' validity (Lewis *et al.*, 2010,
15 2011; Gilewski *et al.*, 2019), utility as a learning tool (Gilewski *et al.*, 2019; Ye *et al.*, 2020), and use as an assessment tool in
16 instructional settings (Trigwell and Sleet, 1990; Ye and Lewis, 2014; Ye *et al.*, 2020). Furthermore, student responses from
17 CEs in general chemistry have been used to generate *Measure of Linked Concepts* true/false assessments that, when
18 coupled with metacognitive activities, were found to enhance student final exam scores (Gilewski *et al.*, 2022).
19 Recently, CEs were also found to be instrumental in revealing the stability of student conceptions of covalent and ionic
20 bonding in a longitudinal study conducted by Bowe *et al.* (2022) in which students completed a CE about SCl_2 and CaCl_2
21 at the end of general chemistry and then again at six months and one year later and found that students consistently
22 incorrectly applied the covalent bonding model to CaCl_2 .

23 In addition to general chemistry, CEs have also been incorporated into biochemistry courses to analyze how
24 students connect chemical and biochemical concepts (Warfa and Odowa, 2015). In their study, Warfa and Odowa (2015)
25 found that students were able to successfully connect foundational chemistry concepts to the biochemical problems
26 when completing the CEs. Similarly, Ngai and Sevan (2018) used CEs in a second semester biochemistry course to
27 evaluate how biochemistry students engaged in chemical identity (CI) thinking to determine how CI is applied in
28 biochemical contexts. They found that the student responses included seven different types of CI thinking. However,
29 while a range of CI thinking was observed, 41% of the responses focused on the CI precursor "composition and
30 structure" in which students provided general observations about the provided substance or molecule, such as
31 degrees of unsaturation or identity of functional groups (Ngai and Sevan, 2018). Finally, Nix *et al.* (2023) explored how
32 biochemistry students approach solving CEs through think-aloud interviews and found that student approaches varied
33 individually and that students completing the CEs in an online course due to the pandemic varied in their approaches
34 from students who, in later years, took the course in person.

35 While used more extensively within general chemistry and biochemistry courses, it has also been incorporated
36 into first-year organic chemistry and upper level analytical and inorganic chemistry courses. For example, within a
37 first-year organic chemistry course, CEs were employed in ungraded group activities to identify which concepts
38 students chose to address and what connections students made between concepts (Mai *et al.*, 2021). In their study,
39 Mai *et al.* (2021) found that students tended to struggle with linking the various chemistry concepts from across the
40 semester since they often did not address previously learned concepts as the semester progressed. In an analytical
41 chemistry course, Wang and Lewis (2020) employed CEs to examine the alignment between student responses and
42 instructor explanations, as well as to assess student ability to explain macroscopic phenomena using submicroscopic
43 statements. Finally, within an inorganic chemistry course, Shaw (2023) found that student CE responses made
44 connections to content from general, organic, and physical chemistry, thus providing evidence of meaningful learning.
45 However, Shaw found that student responses typically fell into either the knowledge or comprehension levels of
46 Bloom's taxonomy with only a few responses reaching the application level (Shaw, 2023) indicating that CEs should be
47 used in conjunction with other assessment types.

48 Currently, the use of CEs in the organic chemistry domain remains largely unexplored, with only one documented
49 instance in a first-year organic chemistry course (Mai *et al.*, 2021). Because upper-division chemistry courses require
50 the application of knowledge acquired from both the current class and the coursework from preceding classes, there
51 arises a crucial need to instruct students on establishing connections not only from within a specific course but also
52 across lower and upper division courses. More specifically, because the concepts in organic chemistry are intertwined
53 and inherently hierarchical, to be successful in organic chemistry, it is essential that students create links between the
54 key organic chemistry concepts. Therefore, we explored the use of CEs as a viable assessment tool for identifying
55 connections that students make in organic chemistry.
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Research Questions

The overall goal of this study was to evaluate the use of creative exercises (CEs) in a *Survey of Organic Chemistry* course through answering the following four research questions:

RQ1. What evidence exists for the validity of the data collected from CEs in a *Survey of Organic Chemistry* course?

RQ2. What connections are organic chemistry students making between concepts in their CE responses? Is there a difference between connections made for high and low-scoring student responses?

RQ3. What student misconceptions about interpreting structures and analyzing organic reactions do CEs reveal?

RQ4. What are students' perceptions of CEs and their contribution to the connections made throughout the semester?

Theoretical Framework

Within prior literature reports, the use of CEs has been grounded in the cognitive constructivist learning theory (Lewis *et al.*, 2010, 2011; Ye and Lewis, 2014; Warfa and Odowa, 2015; Nix *et al.*, 2023). This is because the constructivist perspective specifies that students are not blank slates to be given information, but rather they construct new knowledge by actively integrating that knowledge into their existing schemas. Within the constructivist perspective, Piaget described learning as the interplay of assimilation and accommodation (Kalpana, 2014) where assimilation refers to fitting new information into existing knowledge schemes and accommodation refers to adjusting existing schemes based on new information. Both assimilation and accommodation require students to evaluate how the new information connects to their prior knowledge and schemes (Cakir, 2008). For example, learning about resonance structures, which is the focus of the third CE (CE3) in this study, requires that students connect electron movement and resonance-related structures with prior knowledge about hybridization, electronegativity, the octet rule, charge separation, molecular geometry, and molecular models (Betancourt-Pérez *et al.*, 2010).

To this end, when used as a learning tool, CEs prompt students to identify and build connections between new material and previously learned concepts. This propensity for eliciting connections to prior knowledge is due to both 1) the CE requirement that each response addresses a distinct topic, which promotes the generation of multiple connections, and 2) the CE scoring criteria in which incorrect responses are not counted against the score, allowing students the freedom to be creative in identifying all the connections they make between new and prior material. This promotion of recalling and applying prior knowledge when learning new things in a different context leads to knowledge transfer (Torres *et al.*, 2023) which is an essential step for meaningful learning to occur. Similarly, when used as a consistent assessment tool on exams, it can promote students to think about and identify connections between concepts as they prepare for exams and simultaneously be used as a measure of meaningful learning through counting the number of connections that students make when responding to the CE (Shaw, 2023).

Setting

This study was conducted at a medium-sized, research-intensive university located in the upper Midwest. Data was collected from students ($N = 79$) enrolled in a one-semester *Survey of Organic Chemistry* course offered in the Fall 2019 semester with the approval of the university's institutional review board (Protocol SM20060). All students in the course consented to participating in the study. However, if a student had chosen not to participate in the study, they still could have completed the CEs for bonus points, but we would not have collected their response data for analysis. Because two students dropped the class partway through the semester, their responses for the first exam are included in this study; however, we did not collect responses from them for the rest of the CEs or the *Student Perception of CEs Survey*. Therefore, for CE2 – CE4 and the survey, only 77 students were included in this study. This three-credit course was delivered through two weekly 75-minute sessions for 15 weeks. Commonly declared majors for students enrolled in the course included engineering, animal sciences, biological sciences, agriculture and biosystems, and crop and weed sciences. Furthermore, most students were between their second through final year of degree completion.

This one-semester course used Brown and Poon's 6th edition of the *Introduction of Organic Chemistry* textbook and covered chapters 1-10 and 12-14. Therefore, the following topics were addressed in the course: covalent bonding and shapes of molecules, acids and bases, alkanes and cycloalkanes, alkenes and alkynes, reactions of alkenes and alkynes, chirality, haloalkanes, alcohols, ethers and thiols, benzene and its derivatives, amines, aldehydes, ketones, carboxylic acids, and functional derivatives of carboxylic acids. Overall, student grades were based on three midterm exams (100 points each), a comprehensive final exam (125 points), homework (50 points), and participation in in-class and online assessments and activities (25 points).

This course was held in a SCALE-UP (Student-Centered Active Learning Environment for Undergraduate Programs) classroom (Foote *et al.*, 2016) with 15 round tables and approximately three to six students sitting at each table; students were free to choose where they sat. During the semester, we utilized the Classroom Observation Protocol for Undergraduate STEM (Smith *et al.*, 2013), also known as COPUS, to obtain a COPUS profile of what the instructor and students were doing during the course periods. The COPUS analysis was completed via four classroom observations taken approximately one month apart. The decision to perform four observations was based on the work of Stains *et al.* (2018), in which they stated that, based on their data, at least four observations were necessary for reliable teaching characterization.

The obtained COPUS data was then analyzed using an online COPUS Analyzer tool (www.copusprofiles.org), which indicated that the course was classified as a cluster 5: a student-centered course utilizing a large amount of group work (Stains *et al.*, 2018). During each observation, students were primarily observed listening, working in groups, answering questions, and answering clicker questions. Similarly, the instructor was observed doing real-time writing, lecturing, moving between groups, posing questions, and following up on those questions.

Implementation of Creative Exercises (CEs)

The CEs were incorporated as bonus problems, worth up to five points each, in each of the three course exams and the final exam. Prior to the first exam, students completed one introductory CE (provided in Fig. 1) as an in-class group activity, in which they worked both individually and with their peers at their table. After students completed this introductory CE activity, the instructor led a class discussion on the correctness of the student-generated responses and then provided examples of additional correct responses that had not been mentioned. This first CE was incorporated as a class activity to ensure that all students were familiar with CEs and how to correctly answer them. We did not expect students to have prior exposure to CEs, but because the students came from different disciplines and educational backgrounds, some may have completed CEs previously. However, within the chemistry and biochemistry department at this institution, this was the first course to integrate CEs.

Please write down as many **CORRECT, DISTINCT, and RELEVANT** facts or statements about the following molecules as you can. This is an open-ended question and there are many answers. Please focus your statements on facts that apply directly to these two molecules. (e.g. Stating that carbon has 4 valence electrons may be factually correct but is too general and not relevant to these molecules.)



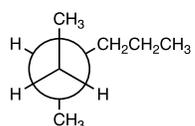
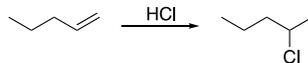
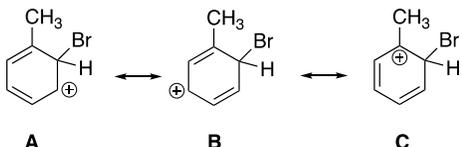
Fig. 1 CE Prompt used in the classroom activity

After learning how to respond to CEs during the in-class CE activity, students then completed a CE on each of the three course exams and on the one final exam. The instructions on all four of the exams were as follows: "Write down five correct, distinct, and relevant facts about [the following]: Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses." (Lewis *et al.*, 2011). A total of four CEs were utilized in the course exams; they are shown in Table 1.

For each test, several students did not complete the CE, thus the reported number (*N*) varies and represents the number of students who attempted each test's CE. While neither author was the instructor for this course, the first author graded the student responses for the CE prompts, and the second author provided feedback and guidance on the grading decisions. The graded responses were then provided to the students when the exams were returned.

Prior to grading the student responses, the responses were first photocopied for future analysis. The obtained responses were deidentified by assigning a randomly generated number for each student that was used in place of their name throughout the semester. The collected student responses were then coded for both topic and correctness by the first author. The assigned codes were then checked by the second author. Any discrepancies in decisions were discussed and resolved.

Table 1 Descriptive statistics of the scores of the CE prompts used on each of the four exams

Exam #	Provided Prompt	Focus of CE	N	M (SD)	Med.	Mode
1		Structure	73	3.41 (1.62)	3	5
2		Reaction	70	3.37 (1.53)	3	3
3		Resonance structure of intermediate	69	2.79 (1.60)	3	2
4		Reaction	73	2.89 (1.52)	3	4

Data Analysis

Examining the relationship between CE scores and exam scores.

Analysis of the quantitative data was conducted using StataC 16 software (StataCorp, 2019). To identify the relationship between the CE assessment score and the overall score of the corresponding exam, the Pearson product-moment correlation coefficients were calculated for each of the CE-exam pairs.

Coding of student responses by topics and correctness.

Student CE responses were thematically analyzed and subsequently grouped with other statements that addressed the same themes. For each CE, a category *miscellanea* was created for unique incorrect, irrelevant, or unclassifiable statements that did not fit into any of the other categories.

Student responses within each category were then classified as *correct*, *incorrect*, *irrelevant*, or *unclassifiable*, consistent with the procedure outlined by Ye and Lewis (2014). A response was given the code *irrelevant* if it was not relevant to the prompt or if the response was not distinct from another prompt that was provided by the student. A response was classified as *unclassifiable* if the statement was too short to identify what the author was trying to convey such as “*Na⁺ masks the negative charge*” for the fourth CE. In this instance, what the “negative charge” is referring to and what is meant by “being masked” is unclear due to the brevity of the statement.

Visualizing connections made between concepts.

To illustrate the connections made between concepts, a visual map for each CE was generated with Gephi software (<https://gephi.org>), using the method reported by Gilewski et al. (2019). To generate each of the Gephi images for the CEs, two files were prepared and uploaded into the Gephi software. The first file contained the information for the nodes and the second file contained the information for the edges. The file for the nodes included the list of topics and the weight for each topic as calculated from the total number of students who mentioned that topic. The file for the edges contained the list of topics and the frequencies of connections between each topic. Within the visual map generated by Gephi, the size of the node corresponded to the number of students mentioning the concept and likewise the width of the edges connecting the nodes corresponded to the number of students who made connections to both of the concepts.

Evaluating student perception of CEs.

To assess student perception of CEs, a *Student Perception of CEs Survey* was administered at the end of the semester after students had completed the first three exams but before the final exam, which contained the last CE. The *Student Perception of CEs Survey* items, illustrated in Box 1, were developed through combining survey items previously reported by Gilewski *et al.* (2019) with two independently prepared survey items. The obtained student responses to the survey items were analyzed using thematic coding, with initial codes based on those reported by Gilewski *et al.* (2019).

Box 1 Student Perception of CEs Survey items

These questions refer to extra credits questions on exams where you are asked to “write down as many distinct, correct, and relevant facts about . . .” We’ll refer to these questions as **Creative Exercises** for the purpose of this survey.

1. Did you attempt to earn extra credit by answering the Creative Exercises questions? If not, what was the primary reason for not attempting to earn the extra credit?
2. Do you think the Creative Exercises helped you make connections among the content in this class? Please explain why you chose the answer for question.
3. How easy did you find it to answer the Creative Exercises?
4. How does this style of questions help you understand chemistry conceptually?
5. Given a choice, would you want Creative Exercises incorporated as part of the assignments and test questions in future courses? You may also want to include any suggested revisions to the Creative Exercises here or on the other side of this page.

Results and Discussion

RQ1. What evidence exists for the validity of the data collected from creative exercises in a *Survey of Organic Chemistry* course?

The validity of the data obtained from CEs has previously been evaluated for both undergraduate general chemistry (Lewis *et al.*, 2011; Ye and Lewis, 2014; Gilewski *et al.*, 2019) and biochemistry (Nix *et al.*, 2023) courses. However, the validity of an item’s data is dependent on both the item itself and the target population. Because these were newly developed CE items and because we wanted to use them with a new target population, students enrolled in a *Survey of Organic Chemistry* course, we first sought to evaluate both 1) evidence based on test content and 2) evidence based on the relationship between the assessment and other variables in order to support the validity of the inferences from the data. These two aspects of validity were chosen for analysis due to their relevance for decisions about future implementations into organic chemistry courses and thus are important considerations for instructors interested in using these CE prompts within their own courses.

Evidence for validity of the data based on the content of the CE. To support the validity of the collected data, prior to administration, the content of each CE was evaluated by two organic chemistry professors, the second author and the course instructor, to ensure that the CEs used were scientifically accurate and had appropriate content coverage and level of difficulty. Both experts agreed that the CEs met the criteria for scientific accuracy and suitable content coverage and difficulty, and therefore no further revisions were necessary.

Furthermore, the authors then compared each CE’s focus with the content of the corresponding exam that was prepared by the course instructor to ensure consistency between the assessed topics. Each 100-point exam contained a series of multiple choice, true-false, and short answer questions along with the extra credit CE. The first exam’s CE (CE1) required that students analyze a Newman projection of an alkane; this was similar to one exam question that required students to identify the relationship between two alkanes that were drawn as Newman projections. The second exam’s CE (CE2) required that students analyze a hydrochlorination reaction of 1-pentene. Likewise, one of the second exam’s questions asked students to predict the product for a hydrobromination reaction. The third exam’s CE (CE3) required that students describe the resonance structures of the intermediate from the electrophilic aromatic substitution (EAS) of toluene with $\text{Br}_2/\text{FeBr}_3$. Similarly, this exam asked students to analyze the EAS reaction of anisole, identify the major product, and circle the most stable intermediate resonance structures. Finally, the CE on the final exam (CE4) asked students to analyze an $\text{S}_{\text{N}}2$ substitution reaction. While this exam’s questions addressed EAS reactions and various addition to alkene reactions, the exam did not directly address $\text{S}_{\text{N}}2$ reactions. However, one question did ask students to assign *R* or *S* configuration to 6 different molecular structures. While not directly asked about on the final exam, substitution reactions such as the $\text{S}_{\text{N}}2$ reaction were taught in the course during the chapter on alkyl halides.

Overall, the developed CEs were found to be of appropriate level of difficulty and were found to be consistent in focus with the test content thus providing evidence for the validity of the data.

Evidence for validity based on the relationship between the assessment and other variables. Convergent evidence refers to how well an assessment relates with other measures of the same construct. To evaluate the convergent evidence of validity for this prompt, the Pearson product-moment correlation coefficients were calculated between the score students received on the CE and that of the corresponding exam, which are provided in Table 2. For each CE, the correlation coefficient indicated a statistically significant moderate relationship between the two scores, thus providing further evidence for the validity of the data.

Table 2 Correlation of CE score to corresponding exam score using Pearson's coefficients (r)

	CE1	CE2	CE3	CE4
N	73	70	69	73
r	0.570	0.396	0.432	0.339
p	<0.0001	0.0004	0.0002	0.0031

When compared to prior studies, the correlation coefficients are similar, albeit slightly lower, in value to those observed by Lewis et al. (2011) for students completing CEs as part of an exam in general chemistry. However, Shaw (2023) observed a stronger correlation between the midterm exam and the CE on that exam for inorganic chemistry ($r = 0.76$); although, in that study the CE was graded as part of the exam, whereas in our study the CE was graded only for bonus points and minimized some students' efforts when completing the CEs which a few students indicated in their survey responses. For example, one student who indicated that the CEs were unhelpful wrote the following in response to whether the CE's helped them make connections: "Not really, by the time I reached the end of the test, I just kind of guessed because I knew it wouldn't hurt me to." Therefore, future studies should explore the impact of scoring methods on the validity of student responses to CEs.

RQ2. What connections are organic chemistry students making between concepts in their CE responses? Is there a difference between connections made for high and low-scoring student responses?

To answer the second research question, student responses were first coded by topic addressed and then grouped with other responses addressing the same theme. A complete list of all coded student responses and their assigned classifications is provided in the supplementary information.

A visual map illustrating connections between the various concepts addressed in all student responses was generated for each CE using Gephi (<https://gephi.org/>). In each of the visual maps, the size of the node for each concept corresponded to the number of students who addressed that topic with larger nodes corresponding to more responses. Similarly, the width of the edges (the line connecting two of the nodes) was proportional to the number of students who addressed both connected topics, with wider lines indicating more students addressed both concepts in their CEs. Although students were not directly asked to make connections between concepts, for students to be able to answer the question, connections between concepts must have been made, even if only subconsciously (Gilewski et al., 2019).

As expected, due to the limited content knowledge at the start of the semester, responses for the first CE (CE1), which prompted students to analyze the structure of an alkane using a Newman projection, exhibited the least number of concepts with a total of 14 different concepts addressed as shown in Fig. 2. CE1 was attempted by 73 students, resulting in a total of 388 responses. The most common topics that students addressed, indicating that they were the most readily available conceptions, included describing the conformation which some students included as multiple responses ($n = 93$, 24%), addressing the atomistic or substituent level ($n = 66$, 17%), addressing the stability ($n = 45$, 12%), and converting to alternative representations ($n = 39$, 10%). Analysis of the edges indicated that the most frequently made connections for this CE included describing the conformation and addressing either its conversion to alternative representations, its stability, or its atomistic/substituent level.

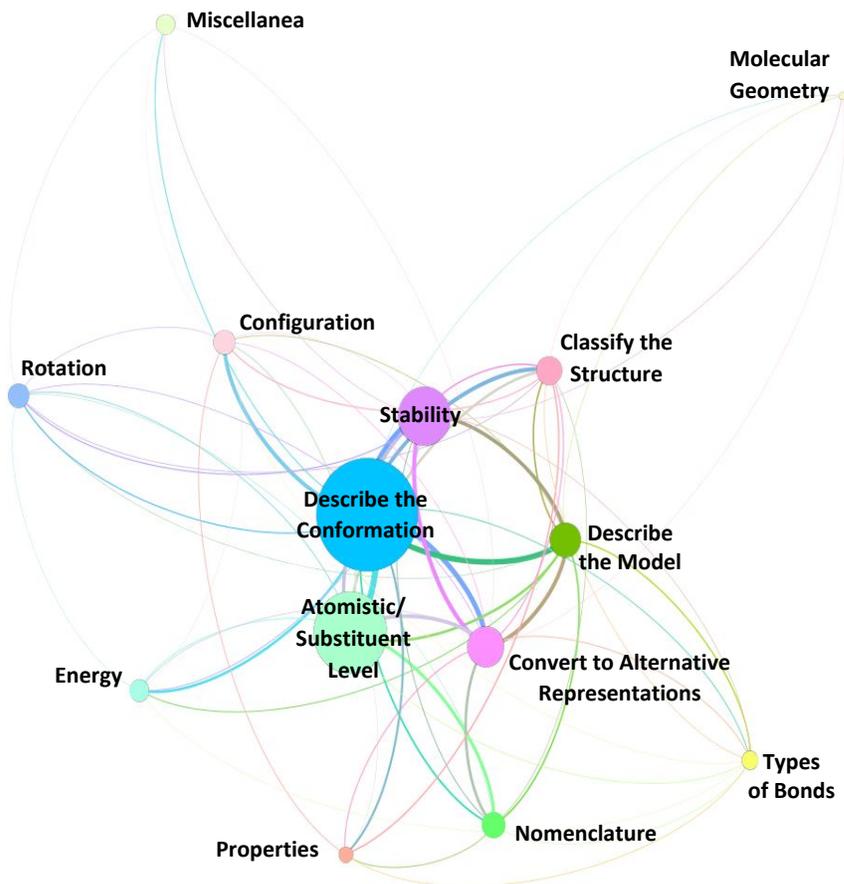


Fig. 2 Visual map illustrating students' linking of concepts observed in the first creative exercise (CE1).

After analyzing the overall connections that students made in CE1, as shown in Fig. S2, we compared the connections that students who scored four or more on CE1 made with those who scored zero to three. We found that correctly describing the conformation of the molecule had the highest frequency in both student groups. Interestingly, only students who provided at least four correct statements addressed the energy of the molecule, and all did so correctly. Finally, it was notable that only students who scored three or less on the CE provided incorrect statements about the types of bonds, the rotation of the molecule, the description of the model, the properties of the molecule, and the molecular geometry of the molecule, and were also the only ones to make incorrect miscellaneous statements.

Subsequently, as illustrated in Fig. 3, responses for the second CE (CE2), which prompted students to consider a hydrohalogenation reaction, garnered a greater number of concepts, with a total of 19 different concepts addressed. CE2 was attempted by 70 students, resulting in a total of 369 responses. The most addressed topics for CE2 included nomenclature of the reactant and/or product ($n = 82$, 22%), classifying the chemical reaction ($n = 59$, 16%), mechanism ($n = 45$, 12%), stereochemistry ($n = 33$, 9%), and addressing the atomistic or substituent level ($n = 23$, 6%). The most common connections between concepts represented by the edges (Fig. 3) were between nomenclature and either classifying the chemical reaction, addressing the stereochemistry, or identifying the mechanism and between classifying the chemical reaction and addressing the stereochemistry.

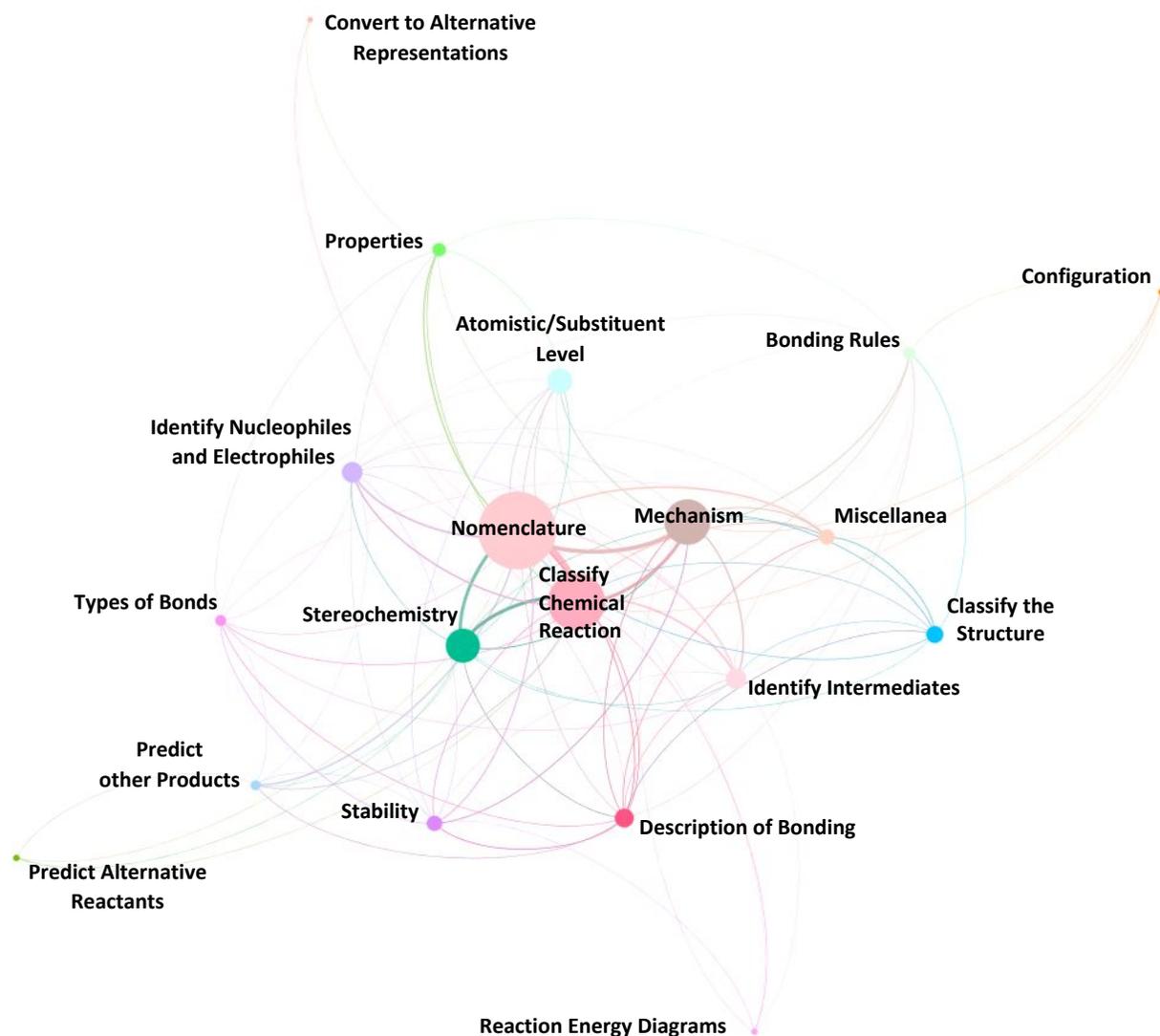


Fig. 3 Visual map illustrating student linking of concepts observed in the second creative exercise (CE2)

Further analysis of the responses from students who scored four or more and those that scored 0-3 on CE2 again indicated differences in their response patterns as shown in Fig. S4. The task with the highest percentage of correct answers from both groups was that of correctly assigning the proper nomenclature to the molecules. However, the starkest contrast between the two groups was in their ability to correctly classify the reaction. While commonly addressed for both groups, 53% of all the students who scored four or more correctly classified this reaction, whereas 53% of all the students who scored zero to three incorrectly classified the reaction as one of their responses. Furthermore, it was observed that only students who scored three or less incorrectly addressed the topics relating to the atomistic/substituent level, the types of bonds in the molecules, the identification of nucleophiles and electrophiles, the bonding rules, the configuration, and the stability and properties of the molecules.

As shown in Fig. 4, responses for the third CE (CE3), which prompted students to consider the mechanistic steps of an electrophilic aromatic substitution reaction (EAS), resulted in the greatest number of concepts with a total of 21 different concepts addressed. Overall, 69 students completed CE3, resulting in a total of 345 responses. The most addressed topics for CE3 included stability ($n = 70$, 20%), arene substitution patterns ($n = 44$, 13%), directing groups ($n = 42$, 12%), resonance structures ($n = 38$, 11%), and addressing the atomistic or substituent level ($n = 28$, 8%).

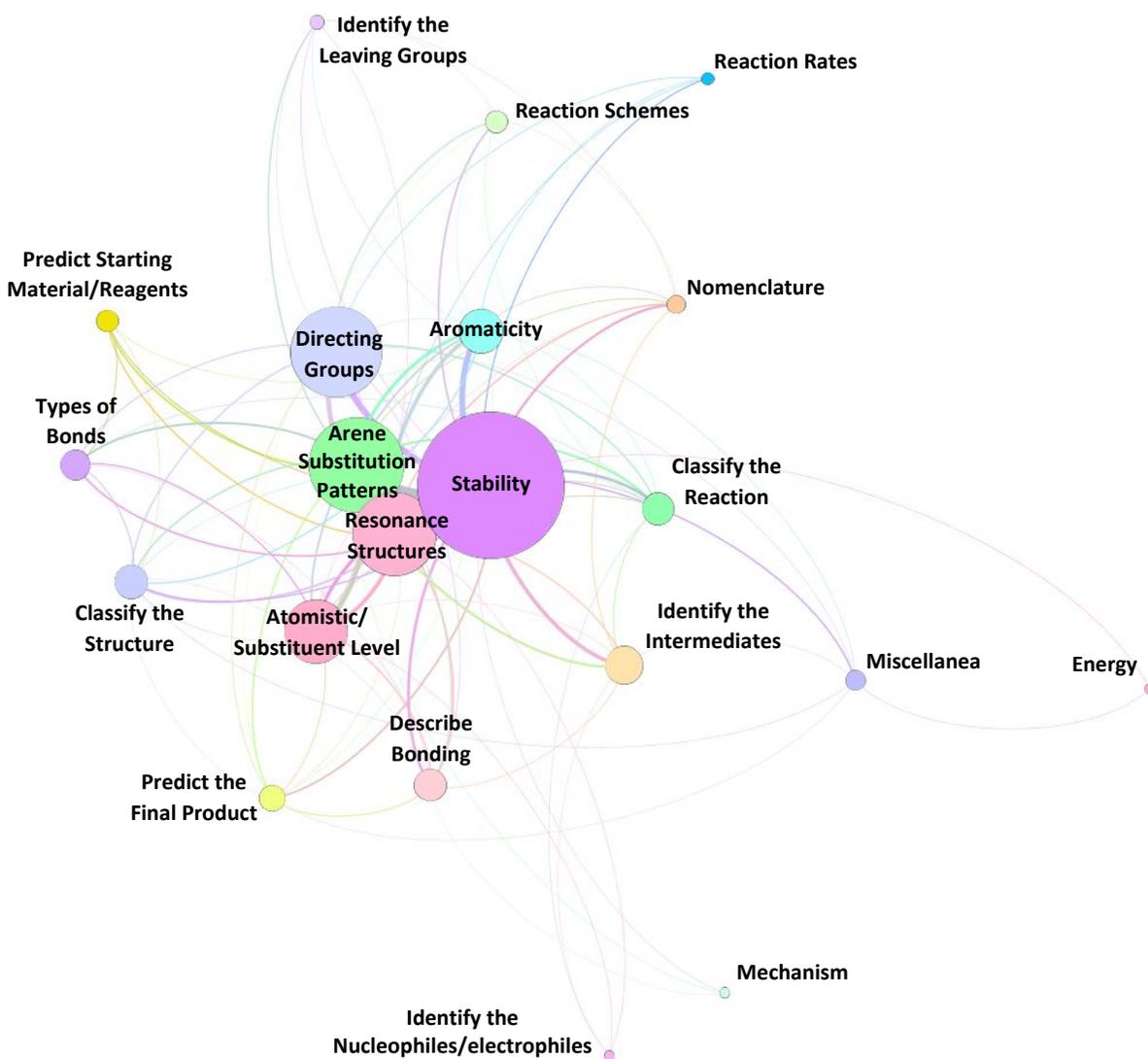


Fig. 4 Visual map illustrating students' linking of concepts observed in the third creative exercise (CE3)

Overall, students tended to score lower on CE3, which is potentially due to its nature of only showing the resonance structures of a reaction's intermediate. There are a variety of literature reports which indicate students struggle with understanding and explaining resonance structures (Betancourt-Pérez *et al.*, 2010; Finkenshaedt-Quinn *et al.*, 2020; Xue and Stains, 2020; Braun *et al.*, 2024) for which student responses towards CE3 provides further evidence.

Therefore, to accommodate this overall lower score, for CE3 student responses were grouped into those that provided at least three correct responses versus those that only provided zero to two correct responses (Fig. S6). Student responses in both groups exhibited the highest rate of correctly addressing the topics of arene substitution patterns, resonance structures, and directing groups. Interestingly, only students that provided at least three correct responses correctly addressed the topic of atomistic/substituent level indicating that although it can be perceived as an easier topic, students still held incorrect conceptions about it, which CEs can help elicit. Finally, it was again observed that only students who scored two or less provided incorrect statements about a variety of topics including the types of bonds, the identification of leaving groups, the description of bonding, reaction schemes, mechanism, energy, reaction rates, and other statements classified as miscellaneous.

Responses for the fourth CE (CE4), which prompted students to consider an S_N2 substitution reaction, resulted in an equal number of concepts as CE3 with a total of 21 different concepts addressed as illustrated in Fig. 5. Overall, 73 students completed CE4, resulting in a total of 352 responses. The most addressed topics for CE4 included classification

of the reaction ($n = 61$, 17%), addressing the configuration ($n = 50$, 14%), addressing the atomistic or substituent levels ($n = 39$, 11%), assigning stereochemistry ($n = 27$, 8%), classifying the structure ($n = 26$, 7%), identifying the leaving groups ($n = 21$, 6%), and providing a description of bonding ($n = 20$, 6%). As shown in Fig. 5, CE4 resulted in the greatest number of edges, indicating that students continued to address a wider range of topics by the end of the semester. The most frequent simultaneously addressed concepts included the classification of the reaction, the configuration, and the atomistic or substituent level.

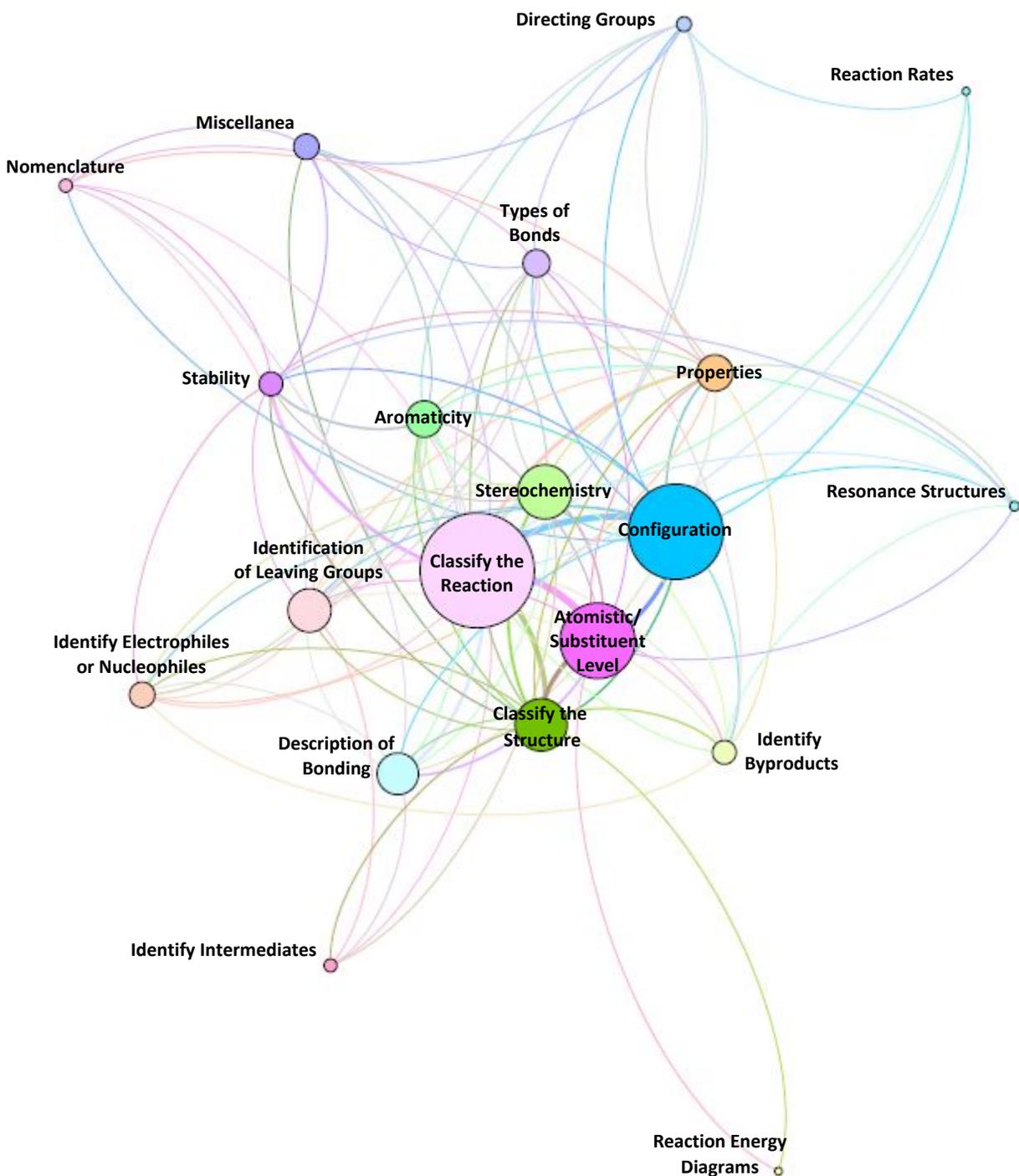


Fig. 5 Visual map illustrating students' linking of concepts observed in the fourth creative exercise (CE4)

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4 Finally, analysis of students scoring four or more and those scoring from zero to three points on CE4 again indicated
5 differences in which topics students chose to address and in their accuracy of addressing those topics (Fig. S8). For both
6 groups the most frequent correctly addressed topics included the classification of the reaction, the
7 atomistic/substituent level, stereochemistry, and the classification of structure. However, only students who scored
8 between zero and three points made connections, albeit incorrect statements, to nomenclature, the mechanism,
9 reaction energy diagrams, and other miscellaneous statements. This may indicate that students who scored lower on
10 the CEs have less developed cognitive structures of this core chemistry content.

11 Overall, the theme of each CE greatly influenced the student responses. However, throughout all four CEs, students
12 frequently identified features to classify or describe at the atomistic or substituent level. This could be due to the
13 associated ease of providing these details or from experience providing similar responses on prior CEs. However, it
14 should be noted that although this concept category is often assumed easier than others, on each of the CEs
15 approximately half of the responses for it were marked as either incorrect or irrelevant, which helped to identify the
16 misconceptions that students possess about these fundamental concepts.

17 **RQ3. What common misconceptions do students in organic chemistry possess?**

18 One key advantage of open-ended prompts, such as CEs, is the ability to probe into student misconceptions that may
19 not surface using close-ended prompts. Thus, to answer the third research question, we analyzed the student responses
20 for each of the CEs for both accuracy and trends in the provided incorrect responses with the complete list of classified
21 statements provided in the supplementary information. Because the prompt was open-ended, the following reported
22 percentages are indicative of the number of students who provided a particular response and are not representative of
23 the percentage of students who may hold that incorrect conception. Therefore, future studies exploring the
24 commonality of these conceptions may be warranted.

25 CE1, which prompted students to analyze the structure of an alkane using a Newman projection, resulted in 388
26 responses from 73 students. Understanding representational models such as Newman projections requires students to
27 develop representational competencies so that they can use representations to think about, communicate, or create
28 meaning about a phenomenon (Kozma and Russell, 2005; Ward *et al.*, 2023). Unfortunately, many students struggle with
29 interpreting the chemical representations (Ward *et al.*, 2023) and preserving spatial relations when translating between
30 representations (Padalkar and Hegarty, 2015). Prior studies assessing students' conceptions about Newman projections
31 found that students struggle with assigning stereochemistry (Mistry *et al.*, 2020), draw incorrect forms of the Newman
32 projection skeleton or use incorrect formulas (Farhat *et al.*, 2019), do not consider the free rotation of the C-C bond and
33 instead consider the structure as fixed (Boukhechem *et al.*, 2011), lack understanding about what the Newman projection
34 represents (Boukhechem *et al.*, 2011), and struggle with translating from dash-wedged notation to a Newman projection
35 when the Newman projection undergoes extensive rotation (Olimpo *et al.*, 2015).

36 Within our study, one misconception observed from CE1 was the application of alkene properties to an alkane
37 molecule by assigning the configuration of the substituents as either *E* or *Z* or as *cis* or *trans*. This was observed in
38 multiple situations including students directly addressing the configuration of the compound ($n = 16$, 22%) or by
39 assigning the configuration within the name of the compound ($n = 2$, 3%). Another misconception, which was also
40 observed in studies by Farhat, Stanford and Ruder (2019) and Ward *et al.* (2023), was that students did not count the
41 carbons that were not explicitly shown in the projection. Thus, students indicated there were only 4 or 5 carbons instead
42 of the expected 6 carbons because they missed counting the carbon denoted by either the front or the back atom or
43 both front and back atoms. This was observed when students provided either the chemical formula or number of atoms
44 present ($n = 8$, 11%), classified the structure ($n = 2$, 3%), and assigned the name of the compound ($n = 2$, 3%).

45 CE2, which prompted students to consider a hydrohalogenation reaction, resulted in 369 responses from 70
46 students. While limited in number, prior studies assessing students' conceptions about hydrohalogenation reactions
47 found that students misclassify them as substitution reactions (Sendur and Toprak, 2013), possess incomplete
48 understanding of resonance structures and the effect of resonance stabilization on carbocation formation (Finkenstaedt-
49 Quinn *et al.*, 2020), may be able to draw the mechanism correctly without understanding the meaning behind the
50 mechanism (DeGlopper *et al.*, 2022), and misuse the term carbocation rearrangement by instead linking it to perceptual
51 attributes such as substituent distribution and functional group changes (Graulich and Bhattacharyya, 2017).

52 The most common misconception observed from CE2 was students identifying the reaction as either an S_N2 ($n =$
53 14, 20%) or S_N1 ($n = 6$, 9%) reaction which is in accordance with findings previously reported by Sendur and Toprak
54 (2013). Additionally, some students again provided incorrect nomenclature when trying to name the compounds ($n = 8$,
55 11%) with several students attempting to assign either the *R* or *S* or *E* configurations to the product ($n = 4$, 6%). Finally,
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another common misconception was that students incorrectly assigned the *R* configuration to the stereogenic carbon ($n = 7$, 10%) which was also observed in the naming of the compound and in their reporting of its configuration ($n = 6$, 9%).

CE3, which prompted students to consider the mechanistic steps of an electrophilic aromatic substitution reaction (EAS), resulted in 345 responses from 69 students. Reaction mechanisms and resonance have been identified as two of the more difficult organic chemistry concepts (Duis, 2011). Prior studies assessing students' conceptions about aromatic compounds found that students view resonance structures as separate oscillating entities (Taber, 2002; Duffy, 2006), think the ring drawn in the structure of benzene indicates there is an electron reservoir inside the ring (Taber, 2002; Carle and Flynn, 2020), and categorize benzene as an alkene (Sendur, 2020). Additionally, a prior study by Duffy that assessed students' conceptions about EAS reactions found that students viewed EAS reactions as an addition of a substituent to the ring instead of as a substitution reaction and identified the reaction as S_N1 because they viewed the breaking apart of bromine as the first step of the mechanism (Duffy, 2006).

For CE3, the most common student misconception was indicating that "intermediate B" was the most stable intermediate ($n = 18$, 26%). Another common misconception was that the students referred to the intermediate resonance structures as products ($n = 11$, 16%). Additionally, students again provided incorrect nomenclature when trying to name the compounds ($n = 5$, 7%) providing incorrect names such as "1-bromo 2 methylcyclohexene" or "1-bromo, 2-methyl, 2,5-cyclohexene." Finally, several students referred to the reaction as S_N1 or E1 ($n = 5$, 7%) instead of as an EAS reaction, a misconception previously observed by Duffy (2006).

Lastly, CE4, which prompted students to consider an S_N2 substitution reaction, resulted in 352 responses from 73 students. S_N2 reactions have previously been identified by organic faculty to be one of the difficult organic chemistry concepts (Duis, 2011). Prior studies assessing students' conceptions about S_N2 reactions found that students often memorize trends for identifying good leaving groups without learning the principles why (Popova and Bretz, 2018; Dood *et al.*, 2020), conflate S_N2 and S_N1 reaction mechanisms (Crandell *et al.*, 2020), associate reaction schemes presented in wedge-dash notation as substitution reactions and reaction schemes in planar notation as elimination reactions (Bucat, 2004; Ladhams Zeiba, 2004), believe that the stereochemistry is conserved during the S_N2 reaction (Cruz-Ramírez De Arellano and Towns, 2014), and assume that the presence of aprotic solvents indicates that an elimination reaction occurred (Cruz-Ramírez De Arellano and Towns, 2014).

Within this study, one of the more commonly observed misconceptions was that the sodium first reacts with the bromine to remove it from the molecule ($n = 8$, 11%). Another common misconception was that DMSO is a catalyst for the reaction ($n = 8$, 11%). As was also observed in the CE1 responses, some students again tried to describe the configuration of the chiral substituent as either *cis* or *trans* ($n = 4$, 5%) indicating the persistence of this misconception. Finally, all students who tried assigning the IUPAC name provided incorrect nomenclature ($n = 4$, 5%) such as naming the reactant "3-bromylcyclohexane" or "R-2-bromo-propane attached to a cyclohexene," suggesting that students continued to have difficulties with naming structures even at the end of the semester.

RQ4. What are students' perceptions of CEs and their contribution to the connections made throughout the semester?

Student perceptions of the CEs were evaluated based on their responses ($n = 52$, 68% response rate) to an end-of-semester *Student Perception of CEs Survey* which is shown in Box 1. Amongst those that responded to the survey, only one student responded in question 1 that they did not attempt the CEs indicating that they focused on the exam instead and therefore their survey response was excluded from the analysis. Among those that indicated they had attempted the CEs ($n = 51$), 37 students (72%) indicated the CEs helped them make connections throughout the course content areas, 5 (10%) indicated the CEs did not help make connections, 8 (16%) indicated the CEs both did and didn't help them make connections, and 1 (2%) indicated that they only guessed on the CEs. For those that indicated it both did and did not help make connections ($n = 8$, 16%) students gave a myriad of reasons such as it helped them remember things but not learn things, that they sometimes guessed or wrote down the things that came to mind most readily, or that it's difficult because if you didn't understand the concepts when first learned it's difficult to apply on future problems. Furthermore, 49 students provided their perceived difficulty of completing the CEs for question 3, with 18 students (37%) indicating they felt the CEs were easy, 20 (41%) indicating they felt the CEs were of mixed difficulty, and 11 (22%) indicating that they felt the CEs were hard.

Student responses ($n = 51$) to questions 2, 3, and 4 (shown in Box 1) were then coded together as having either an overall "helpful" ($n = 38$, 74%), "unhelpful" ($n = 2$, 4%) "both helpful and unhelpful" ($n = 10$, 20%), or "undefined" ($n = 1$, 2%) perception of how completing the CEs impacted their course concept understanding and connections. The

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3 single response classified as “undefined” indicated that the student guessed on the CEs, but they felt that the CEs
4 could have helped them make connections. Responses classified as “helpful” perceptions of CEs ($n = 38$, 74%) were
5 those that found the CEs to either enhance understanding, build connections between concepts, allow for flexibility,
6 or promote metacognition. Responses classified as “unhelpful” perceptions of CEs ($n = 2$, 4%) described CEs as being
7 challenging due to their open-ended nature and not being a specific problem or that they didn’t put enough effort
8 into the class to be able to make the connections. Responses classified as having “both helpful and unhelpful”
9 perceptions of CEs ($n = 10$, 20%) addressed both aspects either in their response to one survey item or addressed
10 “helpful” features in one survey item and “unhelpful” features in another survey item.

11 Using themes originally described by Gilewski *et al.* (2019), student responses classified as “helpful” ($n = 38$) or
12 “both helpful and unhelpful” ($n = 10$) were analyzed together to identify what helpful subthemes they addressed. The
13 resulting subthemes included “knowledge integration” ($n = 38$), “comprehension and awareness” ($n = 19$) and
14 “flexibility” ($n = 17$). Since some students addressed multiple concepts in their responses to the three questions, the
15 combined values for these themes add up to more than the original 48 analyzed responses. Student responses
16 classified as addressing “knowledge integration” described making connections to concepts learned previously in
17 chemistry. These included responses such as “*It makes me understand how most of the material is connected and*
18 *related to each other. All chemistry builds on each other*” and “*it brings all information used on the test and past test*
19 *[sic] into one question.*” Furthermore, responses classified as “comprehension and awareness” addressed students’
20 conceptual understanding of the material. These included responses such as “*I can put two and two together and get*
21 *a better understanding*” [sic] and “*It gives a different way to understand material.*” Finally, responses classified as
22 “flexibility” addressed the benefits of the open-ended nature of CEs and how that open-ended characteristic allowed
23 them to draw on the knowledge that they already have. These included responses such as “*since they weren't asking a*
24 *specific question, it was easier to draw on information previously learned*” and “*the open-endedness gave me a lot of*
25 *freedom.*”

26 To identify what led students to feel that CEs were unhelpful, the student responses classified as “both helpful
27 and unhelpful” ($n = 10$) were further analyzed. Two students indicated that CEs helped them remember concepts from
28 previous chapters, but did not help them learn the material which is warranted since the CEs were administered as
29 part of the exams in this study. Two students indicated it was unhelpful because they would just write down the
30 easiest concepts that came to their mind and another two students felt they were unhelpful because it’s hard to
31 answer the prompt if you don’t understand the chemistry concepts. Both of these responses provide further evidence
32 that CEs have potential for use in identifying learning progressions. In addition, two students indicated that they were
33 unhelpful because they only guessed on the CEs since they were bonus points. Finally, one student felt that
34 sometimes the CEs were hard to understand, and the last student felt it depended on the exam for whether it did or
35 did not help but did not explain why.

36 Question 5 of the survey prompted students to provide their perceptions about whether they would like to see
37 CEs implemented as assignments and tests in their future courses. Of the 49 students who responded to this prompt,
38 22 students (43%) indicated that they would like to see them incorporated in future courses without specifying a
39 preferred method of implementation. An additional 6 students (12%) indicated they would but only as assignments;
40 whereas 2 students (4%) indicated they would but only on tests. Furthermore, another 14 students (27%) indicated
41 they would but only as bonus problems. Finally, four students (8%) indicated that they would not like to see CEs
42 incorporated in future classes and another 3 students (6%) were unsure about whether they would like CEs in future
43 courses. Interestingly, seven students (14%) referenced the impact of CEs on grades as their reason for why CEs
44 should be kept as either bonus points on tests or assignments. This may be due to only requiring five statements for
45 full credit, resulting in each statement accounting for 20% of the points awarded. Due to these student responses,
46 further research on the impact of how CE scores are assigned to student perception of CEs is warranted. Overall,
47 similar to the findings by Gilewski *et al.* (2019), most students viewed the incorporation of CEs favorably and would
48 like to see them implemented in future courses indicating that CEs enhanced their understanding, helped build
49 connections between concepts, and allowed for flexibility in their responses.

50 51 52 **Implications for teaching and research**

53 CEs are open-ended prompts that allow instructors to uncover student conceptions about the course material which a
54 traditional close-ended assessment might not reveal. CEs can serve as a valuable early diagnostic tool for identifying at-
55 risk students or incorrect student conceptions which need to be addressed. In addition, the open-ended nature of CEs
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3 can allow instructors to identify the conceptions students prioritize or have most readily available (Mai *et al.*, 2021),
4 which can be used to help establish student learning progressions. Furthermore, CEs allow students to write out their
5 conceptions about a prompt, providing students an opportunity to practice using the proper chemistry terminology in
6 their response which in turn allows instructors insights into what terms students are grasping and with which they
7 struggle.

8 CEs ask students to identify what they have learned in the course that can be applied to the prompt and do not
9 penalize incorrect connections; therefore, CEs can help support a growth mindset for students. Having students develop
10 and maintain a growth mindset is crucial because whether students have a growth or fixed mindset impacts their
11 persistence, willingness to tackle difficult tasks, and ultimately their academic success (Limeri *et al.*, 2020; Naibert *et al.*,
12 2024; Santos and Mooring, 2024). Similarly, it has been found that student academic performance in organic chemistry
13 has an impact on student mindset with students who struggled in the course shifting towards a fixed mindset (Limeri *et al.*,
14 2020). Thus, using assessments such as CEs which help students see their growth in knowledge and allow them to
15 stretch their conceptions without fear of losing points may be beneficial in supporting their growth mindset.

16 While used as part of the course exams in this study, CEs have also been used in other chemistry education studies
17 as formative assessments via either homework or classroom activities (Gilewski *et al.*, 2019; Mai *et al.*, 2021; Nix *et al.*,
18 2023; Shaw, 2023). When used as formative assessments, it has been reported that the reliability and validity of the data
19 collected by CEs is stronger for in-class CEs than for take-home, which is likely due to students' ability to look up answers
20 for the prompt when not in the classroom (Lewis *et al.*, 2011). Therefore, it is recommended that instructors give special
21 consideration to how they will implement the CEs into their course activities based on the instructional role they wish
22 the CE to fulfill. Finally, to alleviate student concerns when CEs are used as part of a summative assessment, it is
23 recommended that instructors first incorporate the CEs within either group activities or assignments for students to
24 gain experience in how to correctly answer the prompt before the exam.

25 In this study, students scored lower on CE3 which is likely due to the prompt only showing the intermediate
26 resonance structures of an EAS reaction and thus required students to be familiar with both the reaction and its
27 intermediate to be able to provide meaningful statements. Thus, when implementing CEs instructors must be mindful
28 of the complexity of their developed prompts and tailor the content and complexity to fit both the course needs and
29 learning objectives.

30 When creating CEs, it has been recommended that the instructor sets a maximum number of correct statements
31 necessary to receive full credit that is typically one-third to one-half that which the instructor identifies (Ye and Lewis, 2014). Like
32 previous studies, we also found it works best to generate a written list of correct responses prior to grading the CEs and add new
33 correct student responses to the list as they are identified to ease grading and promote consistency of grading especially when
34 multiple graders are grading the CEs. In addition, to minimize grading time for large class sizes, instructors can have
35 students use either self-grading or peer-grading by providing an answer key and then going over it as a class or via a
36 discussion board in case students have responses not already on the key.

37 While CEs allow incorrect conceptions and struggling students to be identified, due to their open-ended nature,
38 they do not indicate how many students hold the generated incorrect conceptions. Therefore, as recommended by Ye
39 *et al.*, instructors can use the student CE responses to generate a *Measure of Linked Concepts* assessment in which
40 students mark each selected student response as either true or false (Ye *et al.*, 2015) which will allow instructors to
41 identify the commonality of the incorrect conceptions. When used in combination with metacognitive activities, the
42 incorporation of these *Measure of Linked Concepts* assessments was found to improve students' final exam scores in
43 general chemistry courses (Gilewski *et al.*, 2022). Therefore, future work should evaluate its impact on students learning
44 within organic chemistry courses.

45 For discipline-based education researchers, CEs are a useful tool for revealing both the conceptions student hold
46 about a topic and the connections students are making between topics. The open-ended nature of the prompts has
47 been found suitable for eliciting students' readily available conceptions about a topic and is quick to administer and
48 evaluate, thus allowing for the generation of responses from many students instead of just a select few as in the case
49 of interviews. The student-generated responses can then be used in the design of a myriad of assessment tools. One
50 key advantage of CEs is that they allow instructors to identify student conceptions with a range of accuracies allowing
51 for the generation of assessments containing distractors with varying levels of correctness. These generated
52 assessments may then be used to measure student learning progressions. Similarly, researchers can provide similar CEs
53 at selected timepoints and conduct a longitudinal study to measure student learning progressions. While CEs have
54 primarily been used within the chemistry education community, further research should explore their modification for
55 other fields to explore student conceptions both within and across disciplines.
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Limitations

There were several key limitations associated with this study which must be acknowledged in order to aid instructors in their decision about whether to implement CEs into their own courses. These limitations include that the study was only conducted at a single institution, not all student responses could be uniquely categorized, the impact of unknown factors on decision to complete the CEs, the potential of student familiarity with completing the CEs being a confounding variable, and the impact of the selected CE topics on the obtained student responses.

Study was only conducted at a single institution

This study was conducted within a single course at one research-intensive institution, and therefore the results may not be generalizable to other settings. Therefore, future studies should investigate its implementation across multiple institution types to allow for further generalization of these results.

Difficulties in categorizing some of the student responses

In this study, because students were not specifically prompted to justify their responses, the depth of their responses varied. Thus, not all statements could be categorized due to the brevity of their nature. We therefore recommend that future implementations explore the impact of requiring students to include a justification for each of their responses to further aid in identifying student conceptions. In addition, student responses sometimes contained both correct and incorrect statements when students provided a more elaborate answer. While we chose to award points for the correct portions, other faculty implementing CEs will need to decide how they wish to handle this prior to assigning the CEs.

Impact of unknown factors on decision to complete the CEs

This study did not explore why some students chose not to complete the CE on the exam. As noted previously, not all 79 students in the course completed each CE. In fact, the completion rate for each of the CEs ranged from 87 to 92%. For each of the CEs it was different students that did not respond, with several students not completing one or two of the CEs. This limits our ability to gain a complete picture of the connections that students were making, since it was typically the lower achieving students who did not complete the CE. Therefore, future studies should both uncover what contextual factors impact students' decisions about whether to complete the CEs and evaluate student responses when the CEs are for course credit instead of bonus points which should enhance the response rate.

Potential of student familiarity of completing CEs being a confounding variable

While we observed an increase in concepts addressed for each CE as the semester progressed which we expect is due to students learning more concepts, it may also be attributed to an increase in student ability to answer the CEs as they became more comfortable with completing them. Furthermore, we did not evaluate whether students have previously completed CEs in their other courses. Although we do know that CEs were not administered within other chemistry courses at our institution, students who participated in this study were from a variety of majors and backgrounds and may have had the opportunity to complete them in their other college or high school courses. Therefore, it is recommended for future studies that students are given multiple opportunities to complete CEs early in the semester to help eliminate the potential for this confounding variable.

Impact of selected CE topics on student responses

In this study, we observed that the topics students chose to address were semi-dependent on the focus of the CE. Since only four CEs were analyzed, we could not evaluate all connections that students were making between the course concepts. Therefore, future studies should incorporate weekly CEs which exhibit a broad range of topics so progress in connections between concepts as the semester progresses can be further evaluated.

Conclusions

In conclusion, in this study CEs were incorporated into a one-semester *Survey of Organic Chemistry* course to identify what connections between chemistry concepts students made and what conceptions students held about the course content. The CEs revealed that the number of topics students addressed for each CE increased throughout the semester, indicating that students were making an increasing number of connections between current and past material. Furthermore, the CEs uncovered that the students held misconceptions about assigning nomenclature and configuration throughout the semester. In addition, it was found that students who scored higher versus lower on the

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3 CEs elicited different connections which may be indicative of their knowledge structures. Finally, students in this study
4 viewed the CEs favorably with most indicating that they would like to see CEs implemented in future courses.
5 Therefore, it is our hope that organic chemistry instructors can use CEs for both stimulating meaningful learning and
6 as an assessment for measuring student learning within their courses.
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8 9 **Ethical Considerations**

10 This study was conducted with approval from the Institutional Review Board (Protocol SM20060) of North Dakota
11 State University and all students consented to participate in the study.
12

13 14 **Data Availability**

15 The data that was used in this study is provided in the Supplementary Information.
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18 19 **Conflicts of interest**

20 There are no conflicts to declare.
21

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Electronic Supplementary Information

for

Utility of creative exercises as an assessment
tool for revealing student conceptions in
organic chemistry

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CE1 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S1 Prompt Provided for CE1

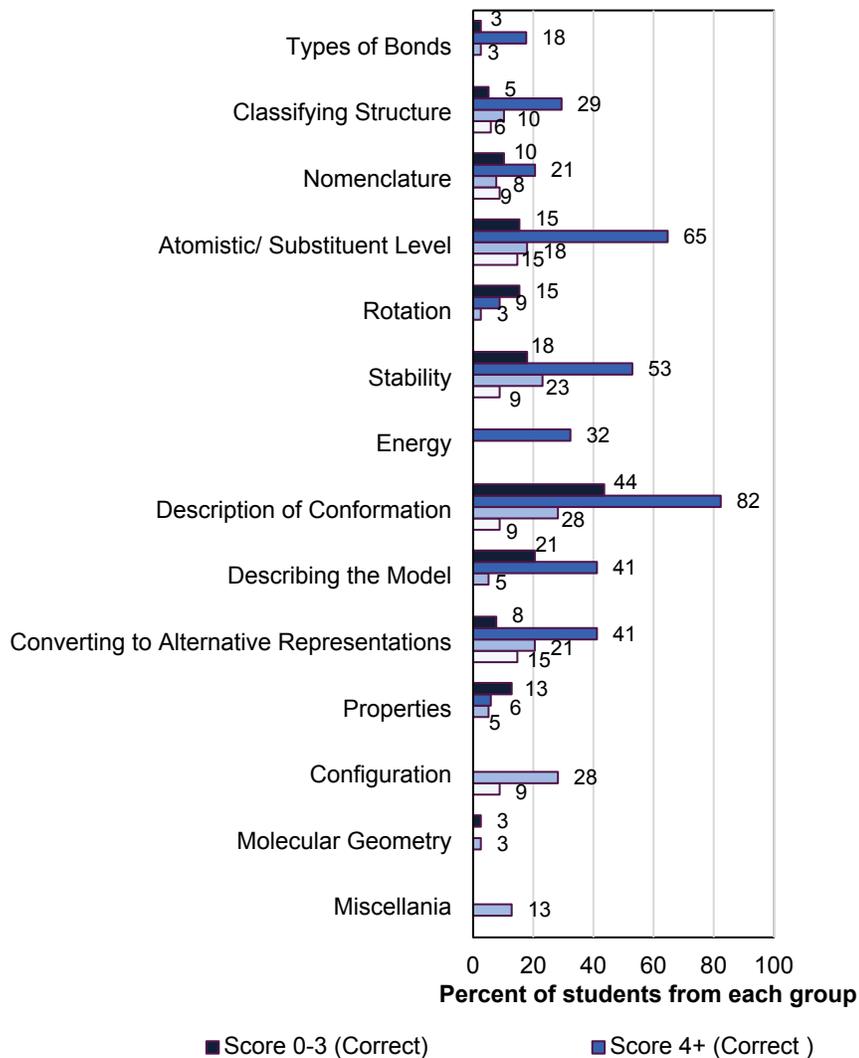


Fig. S2 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE1

CE2 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:

CCCC=C + HCl -> CCC(Cl)CC

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S3 Prompt Provided for CE2

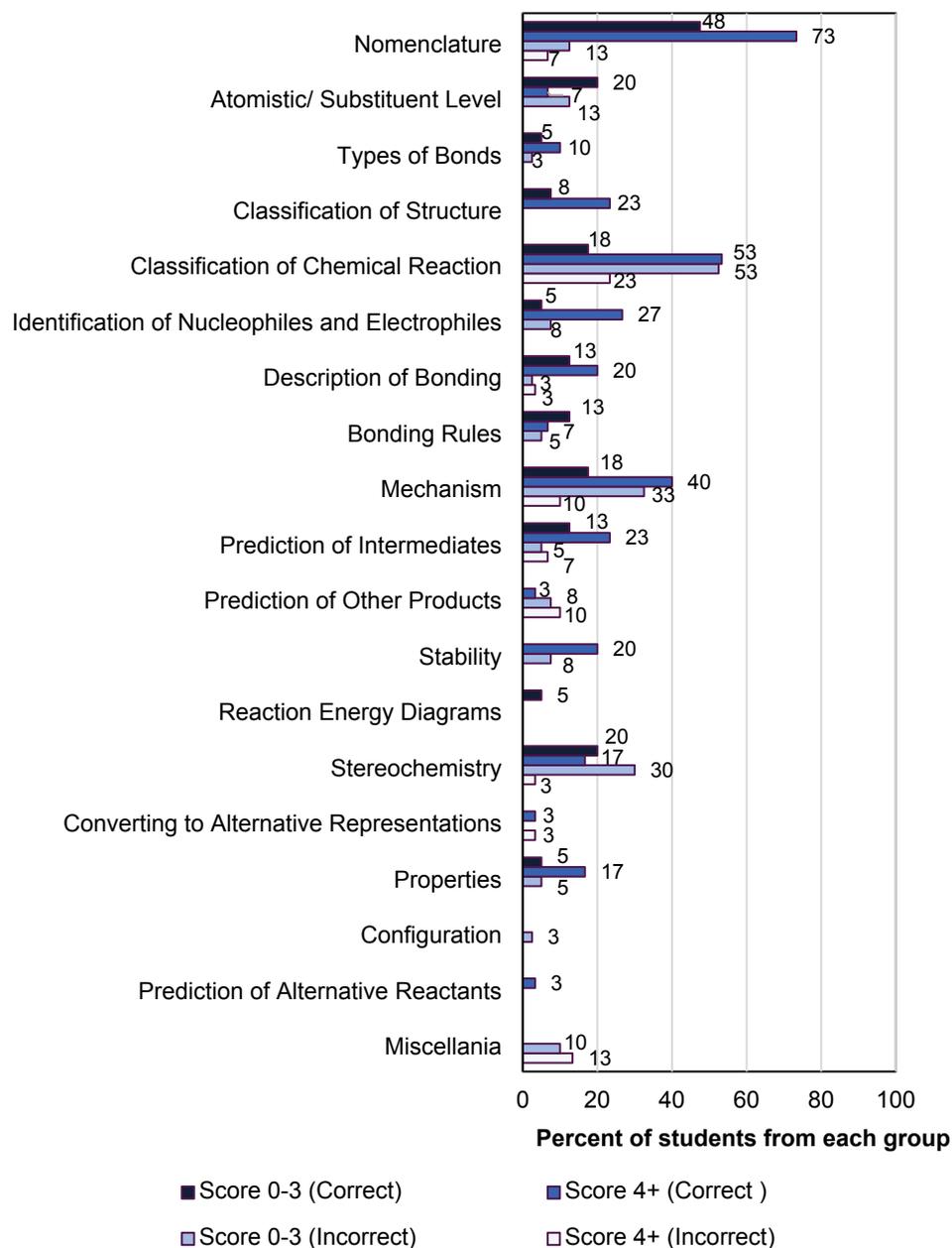


Fig. S4 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE2

CE3 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:

A **B** **C**

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S5 Prompt Provided for CE3

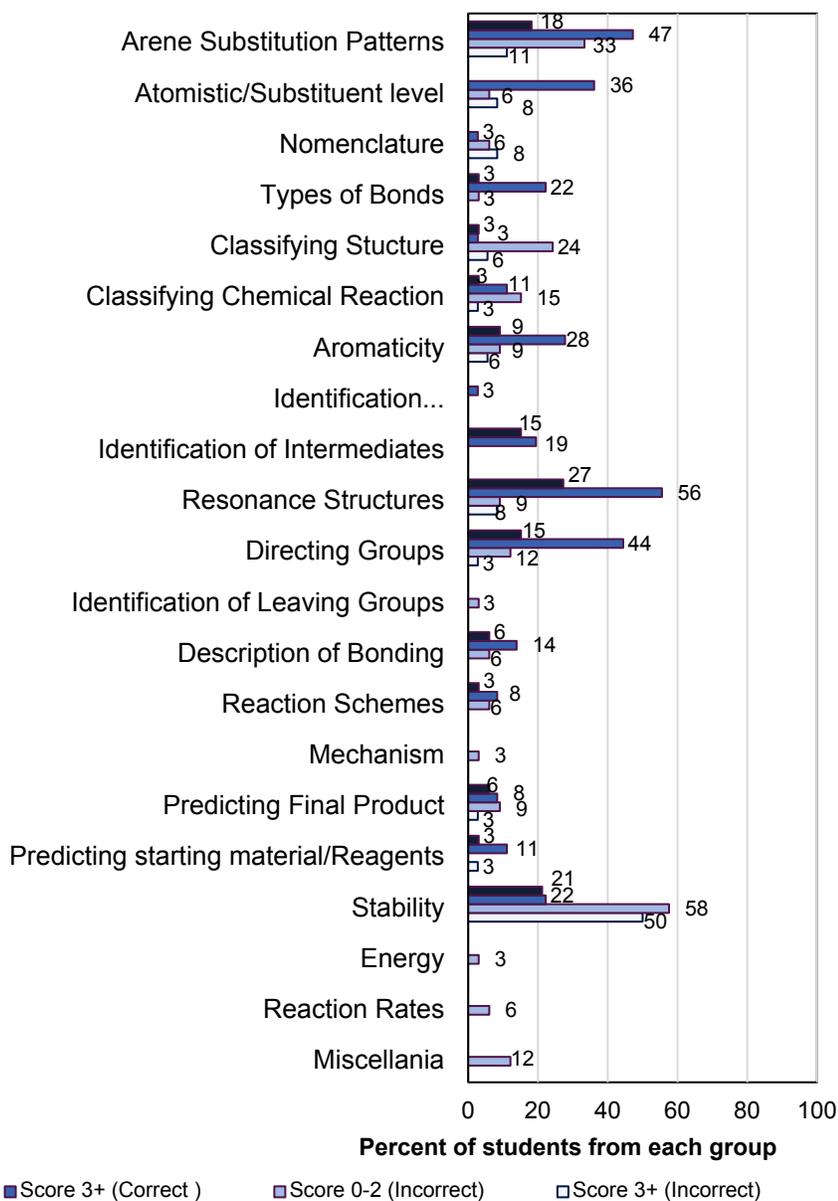


Fig. S6 Percent of respondents in each group, score of zero to two or three or more, who addressed each topic for CE3

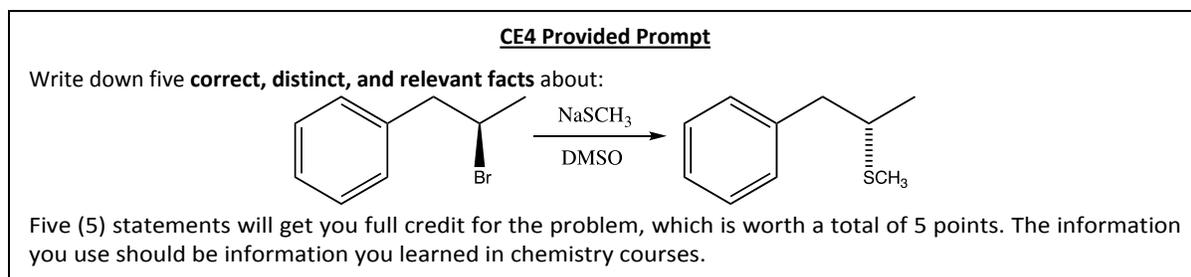


Fig. S7 Prompt Provided for CE4

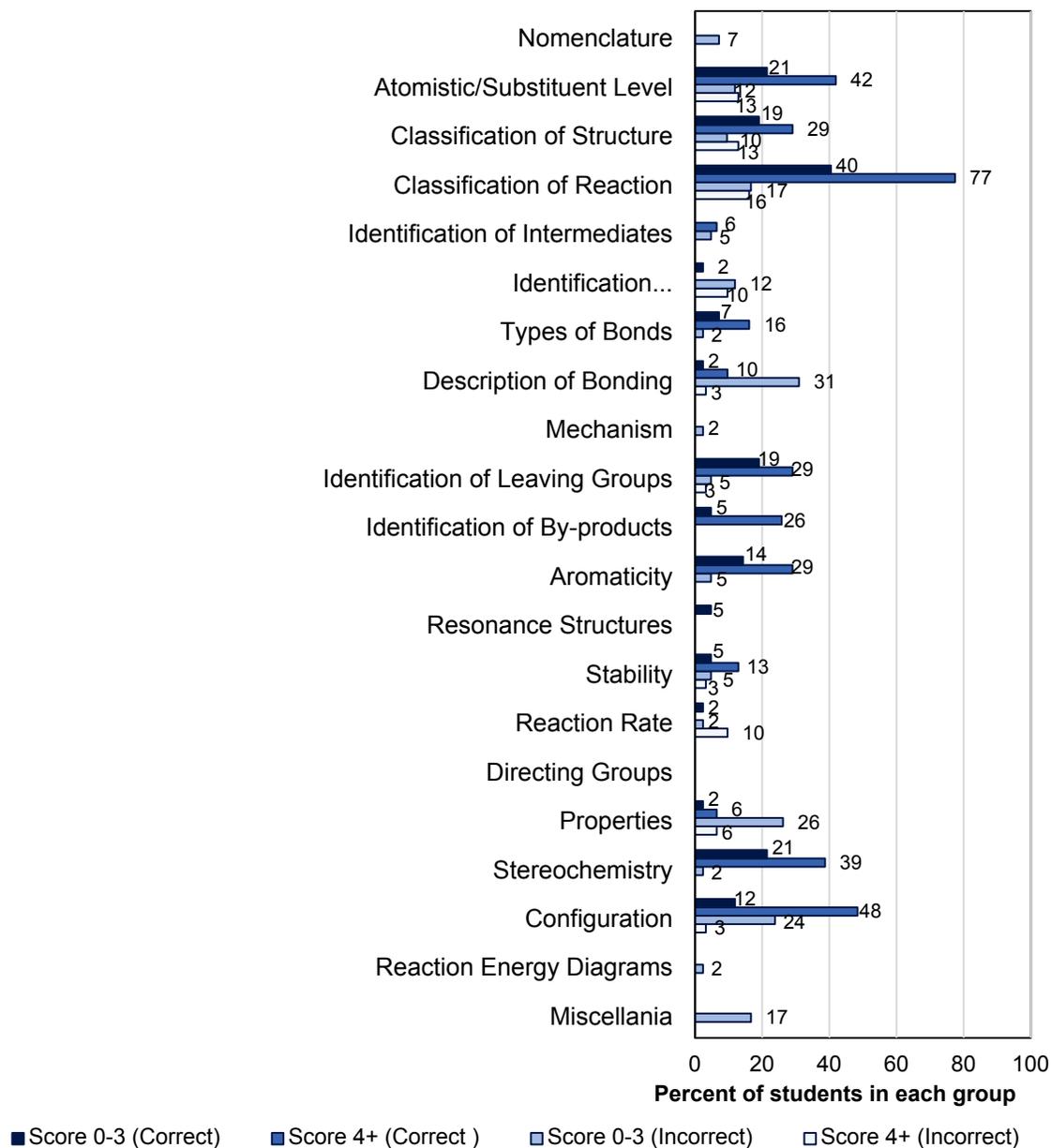


Fig. S8 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE4

Response Classification for Each CE

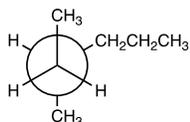
Italics – correct; Bold – incorrect; Bold/italics – irrelevant; Bold/Italics/Underlined - unclassifiable

Values reported in brackets are number of students
Values reported in parenthesis are assigned student code numbers

Creative Exercise 1

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Structure

[11] Types of Bonds

- [2] Molecule contains single bonds that are able to rotate (51, 75)
- [2] The molecule is made up of all sigma bonds that are sp_3 hybridized (11, 14)
- [1] All sigma bonds (62)
- [1] It is saturated (C_NH_{2N+2}) (47)
- [1] All valence shells are filled in this molecule (2)
- [1] There are 3 pi bonds (32)
- [1] Single bonds are made of one sigma bond (13)
- [1] There are no pi bonds in this molecule (9)
- [1] This molecule contains no double or triple bonds (single bonds only) (14)

[20] Classifying Structure

- [10] The molecule is an alkane (2, 6, 9, 20, 25, 36, 42, 47, 49, 60)
- [2] The parent group is hexane (9, 61)
- [2] Diagram depicts a branched alkane (20, 75)
- [1] There are 7 carbons therefore making it a heptane (17)
- [1] This would make this a heptane as $7 \cdot 2 = 14 + 2 = 16$ (53)
- [1] Butane molecule (65)
- [2] Pentane family – 5 carbons (8, 29)
- [1] This molecule is a cyclohexane (32)

[18] Nomenclature

- [12] Its IUPAC name is 3-methylhexane. (11, 13, 14, 25, 27, 31, 38, 41, 47, 62, 76, 77)
- [1] Its name is cis-3-methylhexane. (20)

[2] The IUPAC name for this molecule is 2-ethylpentane. (26, 28)

[1] The name for this molecule is 1,2-methyl-1butylethyl. (22)

[1] The IUPAC name is 2-($CH_2CH_2CH_3$)butane. (65)

[1] Its name is cis-3-methylhex-2-ene. (55)

[1] Stereochemistry

[1] Has stereochemistry (7)

[66] Atomistic/Substituent Level

- [1] The central atom is carbon (60)
- [10] There are 16 hydrogen atoms (10, 14, 20, 22, 34, 46, 54, 67, 75, 78)
- [5] There are 7 carbons (11, 14, 17, 20, 46)
- [1] Six carbons in main chain the other a substituent of the chain (11)
- [2] Has a 6 carbon chain (15, 53)
- [10] Assigned chemical formula as C_7H_{16} (15, 17, 21, 22, 25, 36, 47, 53, 63, 76)
- [4] The molecule has 7 sp^3 hybridized carbons present (28, 31, 38, 76)
- [1] All carbons have sp^3 hybridized orbitals. (13)
- [1] The structure has one propyl group and two methyl groups (45)
- [6] Molecule has 2 methyl groups attached to it (10, 22, 50, 60, 63, 78)
- [2] The molecule contains a propyl substituent (46, 63)
- [1] There is a propyl group branching off the parent chain (36)
- [2] Alkane = $C_NH_{(N \times 2) + 2} \rightarrow C_7H_{(7 \times 2) + 2} \rightarrow C_7H_{16}$ (25, 36)
- [1] It has 0 sp^2 hybridized carbons and 0 sp hybridized carbons present (38)
- [1] Assigned chemical formula as C_5H_{12} (1)
- [1] Assigned formula as $CH_3CH_2CH_2CH_2CH_3$ (8)
- [1] There are 15 hydrogens (52)
- [2] There are 6 carbons (23, 52)
- [4] Molecule contains a total of 5 carbons (34, 54, 75, 78)
- [1] Molecule has 1 butyl group attached to it (22)
- [1] It is an sp orbital (30)
- [1] There is only one sigma bond on this molecule (30)
- [1] There are two sp^2 hybridized carbons present (10)
- [1] There are 6 sp hybridized carbons present (10)
- [1] There are a total of 23 sp^3 orbitals (20)
- [1] Assigned formula as $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ (17)
- [1] There are hybridized carbons present (36)
- [1] The molecule only has carbons and hydrogens (14)
- [1] The shortest possible molecule would equal C_7H_{16} (36)

[16] Rotation

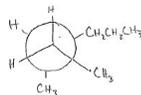
[1] Has different conformers for it (33)

- [8] **Student correctly drew molecule in another conformation (5, 8, 15, 16, 20, 38, 43, 58)
- [5] Molecule contains single bonds that are able to rotate (8, 18, 42, 51, 75)
- [1] Molecule rotates around bond between carbons 4 and 5 (15)
- [1] The molecule can be in any position (38)

Thermodynamics

[45] Stability

- [2] Steric strain between adjacent CH_3 and $\text{CH}_2\text{CH}_2\text{CH}_3$ substituents (6, 18)
- [4] The molecule is not in most stable position (19, 46, 54, 62)
- [2] A conformer of this molecule would look like (this form is less stable than the one above) (43, 57)

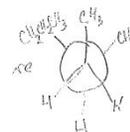


- [9] Staggered is more stable than eclipsed (3, 4, 6, 10, 17, 39, 53, 57, 58)
- [1] There is more steric than torsional strain here (3)
- [2] There is steric strain, especially among the CH_3 and $\text{CH}_2\text{CH}_2\text{CH}_3$ (34, 71)
- [1] This molecule would be experiencing steric strain (28)
- [1] It would be more stable if the $\text{CH}_2\text{CH}_2\text{CH}_3$ was in anti-position because it is a larger molecule (49)
- [2] It would be more stable if the $\text{CH}_2\text{CH}_2\text{CH}_3$ was in anti-position as larger substituent would be less crowded (8, 15)
- [2] The most stable position would be if the $\text{CH}_2\text{CH}_2\text{CH}_3$ was in anti-position (20, 58)
- [1] It is unstable because of the CH_3 being so close to the $\text{CH}_2\text{CH}_2\text{CH}_3$ (68)
- [1] The conformation shown is in the 2nd most stable conformation (76)
- [1] If the back carbon is rotated 60° counterclockwise, it is the least stable conformation (41) [1] If the back carbon is rotated 120° clockwise, it is the most stable (gauche-anti) conformation (41)
- [2] It's a stable molecule (7, 30)
- [1] This state is due to torsional and steric strain (74)
- [1] It is in a staggered conformation which is most stable (49)
- [1] The position of the atoms gives it the least possible torsional and steric strain. (51)
- [1] The front CH_3 and back $\text{CH}_2\text{CH}_2\text{CH}_3$ are gauche resulting in high torsional strain (48)
- [3] It is in the most stable conformation state (18, 29, 74)
- [1] Most stable of the isomers (43)
- [1] Staggered position has more torsional strain than eclipsed position (17)

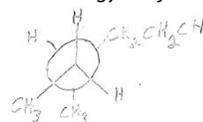
- [1] It's a stable element (59)
- [1] Staggered formation creates torsional strain (23)
- [1] There will be a lot of torsional strain (12)
- [1] This structure is more stable in the eclipse form. (35)
- [1] It is stable (67)

[14] Energy

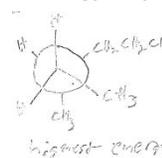
- [7] Staggered is lower in energy than eclipsed (6, 17, 34, 39, 44, 63, 72)
- [1] This formation could gain or lose energy if it was rotated to its conformers (5)
- [1] The change in positions creates different levels of strain which changes the energy (44)
- [1] This structure has less energy than if the staggered were (5, 45)



- [1] This molecule is not in its highest energy state (14)
- [1] The lowest energy conformer is (5)



- [1] This structure has a high energy level due to CH_3 and $\text{CH}_2\text{CH}_2\text{CH}_3$ being closer together. (35)
- [1] The highest energy conformer is (5)



3-D Conformations

[93] Description of Conformation

- [37] The molecule is in staggered conformation (1, 2, 3, 4, 5, 6, 10, 11, 17, 18, 23, 25, 30, 33, 36, 39, 42, 44, 45, 48, 49, 52, 53, 54, 55, 56, 57, 58, 60, 63, 65, 66, 70, 71, 72, 76, 78)
- [3] It is currently in gauche conformation (41, 74, 76)
- [12] CH_3 and $\text{CH}_2\text{CH}_2\text{CH}_3$ are in gauche position (1, 3, 4, 5, 25, 46, 48, 49, 55, 54, 61, 70)
- [6] The top CH_3 is 60° from the $\text{CH}_2\text{CH}_2\text{CH}_3$ (39, 55, 56, 60, 66, 72)
- [10] Top and bottom CH_3 are anti to each other (3, 4, 19, 48, 49, 55, 54, 56, 61, 70)
- [4] Methyl groups have 180° between them. (12, 55, 65, 72)
- [1] Can have conformational isomers (13)
- [1] The front CH_3 and back $\text{CH}_2\text{CH}_2\text{CH}_3$ have a gauche staggered (66)

[2] The molecule is not in the eclipsed position (9, 34)

[1] There is one anti-staggered gauche position in this conformation (9)

[1] The carbon at the 12:00 and the carbon at the 6:00 are in linear conformation (46)

[1] Bond angles are 109° (13)

[1] Bond angles are 109.5° (60)

[1] The relationship between CH_3 on the back carbon and $\text{CH}_2\text{CH}_2\text{CH}_3$ is anti (70)

[1] The bond angles are all at 60° (51)

[1] The front CH_3 and back CH_3 are anti-gauche staggered (66)

[1] One methyl and the only butyl group are gauche to each other (19)

[3] The bond angles are 120° apart (32, 36, 71)

[1] The bond angle is 180° . (30)

[1] The bond angle between the front CH_3 and back CH_3 is 180° . (66)

[1] Eclipsed (19)

[1] Methyl groups are in gauche position (12)

[1] The element is staggered (59)

[1] The following is an example of the molecule in a staggered conformation (42)



[1] It is a conformer (38)

[1] This is a conformation (44)

[1] This molecule can conform (31)

[1] 1 gauche, anti-staggered (62)

[25] Describing the Model

[20] This is called Newman's projection (4, 9, 11, 17, 19, 23, 28, 45, 47, 49, 51, 55, 56, 66, 69, 71, 72, 74, 75, 76)

[1] You rotate the bottom half to create different conformations (35, 44)

[1] This projection is the one that looks at the molecule from one and over the main carbon-carbon bond (35, 51, 57)

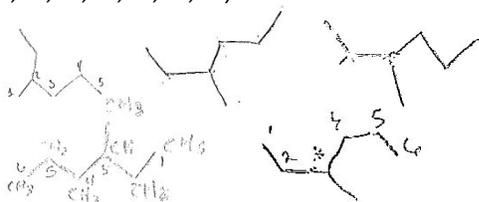
[1] Conformers are easy to be found using this model because it is simply rotating (35)

[1] Shown in the face of a sawhorse model (67)

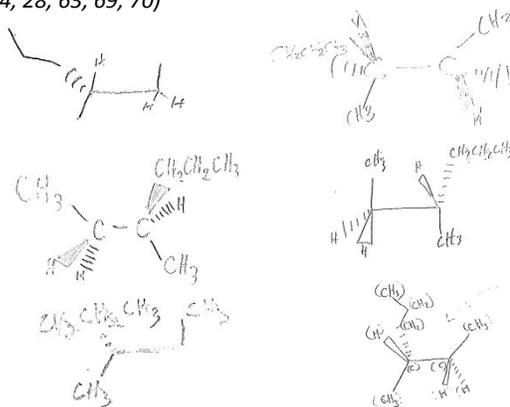
[1] It is a seahorse model (58)

[39] Converting to Alternative Representations

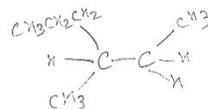
[10] **Correctly redrawn using a line structure (11, 13, 14, 20, 26, 27, 28, 47, 57, 76)



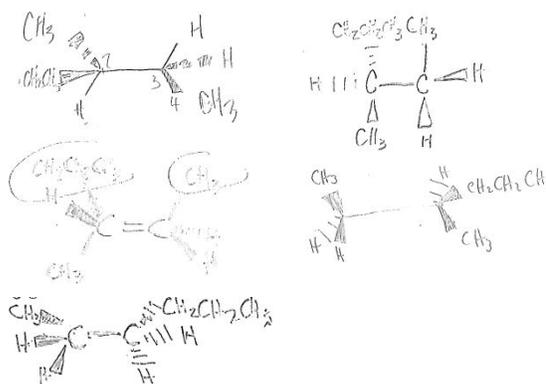
[7] **Correctly redrawn using wedge and dash notation (5, 9, 14, 28, 63, 69, 70)



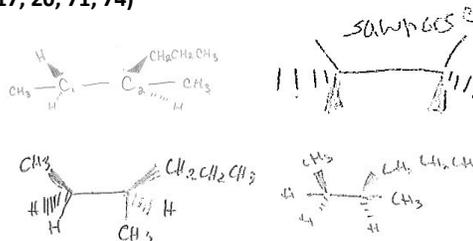
[4] **Correctly redrawn using a Kekule structure (2, 53, 62, 76)



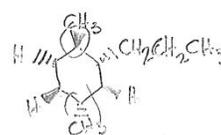
[5] **Incorrectly redrawn using wedge and dash notation (33, 35, 50, 55, 65)



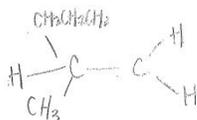
[4] ** Incorrectly redrawn as a sawhorse projection (17, 20, 71, 74)



[1] **Incorrectly redrawn using flat ring structure (50)



[1] ****Incorrectly redrawn as a Kekule structure (19)**



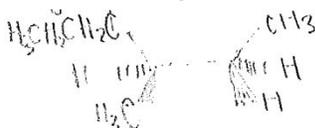
[3] **** Incorrectly redrawn as a line structure (8, 10, 28)**



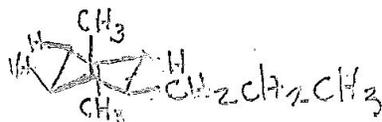
[1] This is the sawhorse projection when viewed from the eye labeled 5. (41)



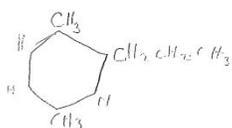
[1] The seasaw diagram would look like (51)



[1] This molecule can be drawn as a chair structure (50)



[1] It can be a cyclohexane if drawn like that (59)



[10] Properties

[1] It would need an extremely strong base to deprotonate it (53)

[1] This molecule is non-polar (2)

[1] This molecule would be a liquid at room temperature (31)

[1] It is liquid at room temperature due to having more than 4 carbons (27)

[2] It is a weak acid (32, 67)

[1] Molecule likely behaves as an acid (65)

[1] This molecule is less acidic than water (2)

[1] It is highly reactive (69)

[1] $\text{CH}_2\text{CH}_2\text{CH}_3$ is the strongest acid (61)

[16] Configuration

[5] It is trans (32, 33, 50, 67, 78)

[4] It is a cis isomer (12, 20, 42, 61)

[1] The two CH_3 s are cis (58)

[1] This molecule has a cis bonding structure (31)

[4] It is in a Z formation (5, 42, 53, 70)

[1] Sits at an E – configuration (33)

[2] Molecular Geometry

[1] Tetrahedral shape (29)

[1] The original molecular geometry is sawhorse. (71)

[12] Miscellanea

[1] They are stereoisomers. (12)

[1] It would have the most torsional strain when it moves to the boat position (59)

[1] It is in chair formation (7)

[1] Both the CH_3 are more electronegative than the $\text{CH}_2\text{CH}_2\text{CH}_3$ (18)

[1] Constitutional isomer (moving atoms) (59)

[1] The Anti-methyl groups are [unreadable] to the same carbon (12)

[1] Evenly placed (40)

[1] Balanced (40)

[1] If linear $\text{C}_N\text{H}_{2N+2}$ (29)

[1] If cyclo C_NH_{2N} lose 2 H because of the circular shape (29)

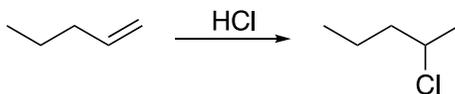
[1] Is an isomer (7)

[1] Is not in resonance form (7)

Creative Exercise 2

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

[82] Nomenclature

- [29] The starting molecule's name is pent-1-ene (4, 5, 8, 11, 13, 14, 15, 16, 17, 19, 20, 22, 25, 31, 33, 38, 41, 42, 45, 50, 51, 55, 57, 59, 60, 65, 70, 77, 79)
- [6] Reactant is 1-pentene (2, 27, 46, 54, 71, 74)
- [34] The product is 2-chloropentane (4, 5, 8, 11, 13, 14, 15, 16, 17, 19, 21, 22, 25, 27, 29, 30, 31, 33, 36, 42, 45, 46, 50, 51, 55, 56, 57, 58, 59, 60, 61, 65, 71, 74)
- [4] The other starting material is hydrochloric acid (14, 15, 27, 74)
- [1] The starting material is pent-2-ene (30)
- [1] The product molecule's name is 2-chloralpentane (38)
- [1] The product is (S)-2-chloryl-pentane. (26)
- [2] The product is (R)-2-chloropentane (63, 70)
- [1] The product is called 1-chloropentane (20)
- [1] The product is 4-chloro-pentane (53)
- [1] (E)-1-chloropentane is the product (10)
- [1] The pent-1-ene react with HCl (79)

[23] Atomistic/Substituent Level

- [1] Cl is 2° (52)
- [3] Cl is connected to a secondary carbon (29, 32, 74)
- [4] Both compounds have 5 carbons. (15, 22, 34, 67)
- [1] Reactant has 5 carbons (32)
- [1] The chemical formula is C₅H₁₁Cl (53)
- [1] There is one methyl group in the first molecule (78)
- [1] The starting compound has 11 hydrogens (32)
- [1] There are two ethyl groups in the second molecule (78)
- [1] Cl attaches to a 3° carbon (8)
- [1] The substitution takes place on a 2° section of the molecule (5)
- [1] There is only one off branch present (67)
- [2] Cl is a halogen (49, 72)
- [1] The starting compound has 10 hydrogens (34)
- [1] The ending product has 1 chlorine (22)
- [3] The ending product has 11 hydrogens (22, 32, 34)

[7] Types of Bonds

- [3] It contains one pi bond (double bond) (34, 49, 60)
- [2] The product is composed of all sigma bonds (2, 6)
- [1] There is a tertiary bond (67)
- [1] HCl is bonded with a covalent bond (25)

[14] Classification of Structure (Reactant/Product)

- [6] The reactant is an alkene (6, 17, 41, 47, 60, 66)
- [2] Product is an alkane (17, 60)
- [3] It starts out as pentene (32, 58, 61)
- [3] Product is an alkyl halide (47, 55, 75)

[59] Classification of Chemical Reaction

- [11] This is an addition reaction (9, 20, 28, 45, 49, 50, 51, 57, 62, 65, 76)
- [1] + HX addition (63)
- [6] This is a hydrohalogenation reaction (2, 3, 49, 51, 62, 75)
- [1] Halogenation reaction (13)
- [1] This is a hydrochloronation reaction (14)
- [3] It will be an exothermic reaction (19, 28, 81)
- [1] The reaction seems to be an acid-base reaction (45)
- [5] 2-step reaction (2, 21, 26, 27, 76)
- [1] It is an electron rearrangement (81)
- [1] A substitution takes place between the reactant and the product (20)
- [1] Nucleophilic substitution (53)
- [12] It is SN₂ substitution (10, 18, 19, 25, 28, 29, 33, 38, 56, 61, 62, 70)
- [2] This is an SN₂ because it is only one step (1, 59)
- [3] This is a one-step reaction (33, 56, 71)
- [6] This is a SN₁ substitution (5, 8, 46, 55, 65, 66)
- [1] It is an endothermic reaction (36)
- [2] Reaction is a hydration reaction (16, 26)
- [1] Beta-elimination reaction (75)

[18] Identification of Nucleophiles/Electrophiles

- [1] HCl is an electrophile (6)
- [7] Chlorine is acting as the nucleophile (4, 8, 10, 14, 20, 21, 28)
- [1] Cl⁻ is a good nucleophile (51)
- [1] H⁺ is the electrophile (21)
- [1] The H is the electrophile (20)
- [3] The alkene is a nucleophile (6, 47, 66)
- [1] 1-pentene is an electrophile (54)
- [1] HCl is a nucleophile (54)
- [1] HCl is a weak nucleophile (5)
- [1] Cl is the electrophile (77)

Bonding**[16] Description of Bonding (Breaking/Forming)**

- [2] Adding HCl to the starting group breaks the pi bond (30, 32)

[1] Pi bond breaks forming a positive position in the 2 position. (25)

[1] The reaction between electrophile and nucleophile to form new covalent bond (39)

[1] In the reaction of alkene, pi bond is broken and, in its place, sigma bonds are formed (39)

[1] pi bond broken to form a new single bond (75)

[1] Nucleophile (Cl^-) is reagent that donates unshared pair of electrons to form the new covalent bond (39)

[1] The chlorine bonded to the most stable carbocation (41)

[1] Double bond breaks when HCl added (19)

[1] The double bond breaks in this reaction (13)

[1] The first step is the pi bond breaking (46)

[1] Carbon double bond goes away (58)

[1] HCl is also breaking its bond, separating H and Cl so that HCl is not in the products (47)

[1] The double bond breaks in this reaction, forming a bond with Cl (47)

[1] The breaking of bond to make stable ion or molecule (39)

[1] The double bond relocates (67)

[9] Bonding Rules

[1] Cl will bond to the carbon with the least amount of hydrogen bonds (35)

[1] Cl will always bond to the more substituted carbon (36)

[1] The hydrogen will attach to the carbon on the end because it has the most hydrogens when the double bond is broke (54)

[1] This follows Markovnikov's principle, H adds to the rich side (3)

[1] This follows Markovnikov's rule, Cl is added to the most substituted carbon (9)

[1] This reaction follows Markovnikov's rule (48)

[1] This is a Markovnikov reaction (41)

[1] The Cl is happy because it is attached to the bottom of where the double bond was (61)

[1] Doesn't have regioselectivity (18)

Mechanism

[9] Complete Mechanism

[2] This reaction will form a carbocation (18, 48)

[1] This is a multistep reaction, where first the double bond breaks and a + charge appears. (66)

[1] The reaction has 2 steps, the protonation of the substrate and the chlorination of the substrate (14)

[1] Reaction takes place via 2 steps, first leaving group leaves and creates a carbocation intermediate, then secondly the halogen attaches to the carbocation (55)

[1] The positive charge moves from being a primary to a secondary. (66)

[1] No rearrangement will occur due to it already being most stable at 2°, no option for 3° (3)



[1] The arrows would push like this: (20)



[17] First Mechanistic Step: Addition of Electrophilic H^+

[1] The first step, the hydrogen adds to end of chain breaking double carbon (74)

[1] The H becomes an H^+ and takes the double bond's electrons and gives the 2nd carbon from the right a + (18)

[1] The H^+ breaks the double bond resulting in formation of carbocation (15)

[1] Hydrogen from HCl breaks the double bond (17)

[2] The hydrogen gets rid of the double bond (56, 61)

[1] Addition of the H molecule gets rid of the double bond (33)

[1] The hydrogen on HCl connects to the carbon on the end of the double bond (58)

[1] The pie bond of the starting material is broken and its electrons are transferred to H of HCl. (11)

[2] The double bond gets protonated in the reaction (13, 14)

[1] This reaction involves protonation of 1-pentene by HCl. (2)

[1] In the first step of this reaction the H^+ from HCl reacts with the double bond of the first molecule and Cl^- is left off (42)

[1] HCl will donate its proton to the right side of the double bond which will then break (48)

[1]  (73)

[1] The hydrogen helps break the double bond (72)

[1] Chlorine breaks the double bond (31)

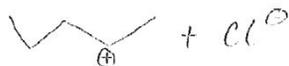
[10] Second Mechanistic Step: Addition of Cl^-

[1] HCl splits leaving H^+ and Cl^- . Cl^- moves in and bonds to positive charged C (15)



[1] The Cl^- formed from protonating the starting materials bonds with the carbocation to form the product. (11)

[1] After the double bond is removed, before the Cl is added the molecule has a positive charge on it (72)



[1] The chlorine is attached where it is to get rid of the charge and make

molecule neutral (56)

[1] The Cl is a - after the H and it bonds with the + on the carbocation (18)

[1]



The nucleophile attacks the plus charge in

the molecule to

make the product (4)

[1] During the 2nd step, Cl bonds to C₂ (76)

[1] (73)

[1]



Cl takes over the

electrons from the broken double bond (30)

[1] The bridging intermediate blocks off the one side of the molecule so that is why the Cl had to bond on the bottom (49)

[9] Incorrect Mechanistic Steps

[1] (73)

[1] When the double bond is broken, the carbons are left with positive charges. The hydrogen bonds with one of the carbons, eliminating one of the positive charges. When hydrogen breaks from Cl, it leaves Cl with a negative charge. Cl bonds with the other positively charged carbon (35)

[1] The alkene breaks to an alkane leaving excess charges so HCl can bond to it (9)

[1] The double bond is removed to a charge, then Cl is added on (52)

[1] First step in reaction is to break double bond, leaving an electron poor spot for the Cl to attack as it has a negative charge on it (3)

[1] The double bond is broken with HCl creating a H₂ molecule and Cl⁻. The Cl⁻ is attached then after to the 2nd carbon on the chain (22)

[1] The pi bond, where there is a double bond, breaks. This breakage creates a plus charge at the 2nd carbon.

The negative Cl forms a bond with the plus charge (79)

[1] This is a multi-step reaction where first the double bond breaks and positive charge appears. After the first step of breaking the double bond, we have a carbocation. Carbocation rearranges the positive charge before the Cl⁻ attacks to be more stable (66)

[1] First step is to break the double bond (81)

[18] Predicting Intermediates

[10] The following is the intermediate step (15, 16, 38, 41, 48, 58, 63, 72, 73, 76)

[1] (two intermediates) (21)

[1] Before chlorine bonds, there is a second degree (2°) carbocation in the intermediate (41)

[1] After the first step of breaking the double bond we have a carbocation (66)

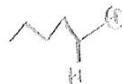
[1] Intermediate A will be a 2°, intermediate B will be a 3° carbocation (81)

[1] It creates a bridging intermediate (49)

[1] There will be 2 intermediates (81)

[1] This reaction wouldn't have any intermediates (50)

[1] The intermediate carbocation will likely look like (6)



[6] Prediction of Other Products

[1] A minor product could be 1-chloropentane (27)

[1] A positive H⁺ molecule is a byproduct of the reaction (46)

[2] No minor products (25, 31)

[1] There could be a product where Cl is on another carbon [student drew examples illustrating on C1 or C3] depending on if the carbocation relocates and where it relocates to (41)

[1] An expected product may be but it's not because with Cl being attached to a 2° carbon is more stable than 1° carbon (20)

[11] Stability

[2] More substituted carbocation are more stable (20, 39)

[1] Cl bonds to carbon 2 because it's 2°, whereas carbon 1 is 1°, 2° is more stable (76).

[1] The carbocation will form on the 2° carbon because it is most stable (11)

[2] The final product is more stable (2, 74)

[1] A stable reaction because of the location of the Cl (53)

[1] In this form, the reactant is most stable (32)

[1] The product is a 2°, making it more stable than the reactant (1)

[1] The addition of HCl makes the product less stable than the reactant (33)

[1] The reaction is stable (67)

[2] Reaction Energy Diagrams

[1] Its energy diagram should look like the energy diagram below where the arrow labeled b indicates the rate determining step and the middle, labeled A is the intermediate step (38)



[1] The graph would be exothermic, as energy of products is lower than energy of reactants (1)



[33] Stereochemistry

[7] The product contains a stereogenic carbon (54, 55, 62, 63, 70, 71, 78)

[3] The starting material contains zero stereogenic carbons (30, 63, 70)

[1] If the H is facing down it would be R. If the H was facing up it would be S. Using Cl as our stereochemistry (59)

[1] The Cl group is not stereospecific as it can go either on the front or the back (3)

[3] The product is chiral (28, 55, 65)

[1] Product contains 0 planes of symmetry (55)

[1] There is no plane of symmetry (52)

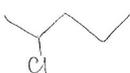
[1] There are no stereogenic carbons in the product (30)

[6] The stereogenic carbon has an R configuration (46, 54, 62, 63, 71, 78)

[1] This molecule is chiral (31)

[1] Chiral (29)

[1] Both molecules are chiral (56)

[1]  would be the enantiomer/mirror image for the product (10)

[1]  would be a diastereomer for the product. (10)

[1] Product is achiral (8)

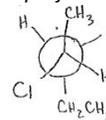
[1] Enantiomers (29)

[1] The molecule is stereogenic (7)

[1] It's non-meso. (50)

[1] Converting to Alternative Representations

[1] This is another projection of the product (57)



[10] Properties

[4] HCl is a strong acid (15, 34, 42, 57)

[1] HCl is an acid (78)

[1] The reaction occurs in an acid (hydrochloric) (14)

[1] This wouldn't require a catalyst because the HCl is strong enough to break bonds (50)

[1] HCl also acts as a catalyst (36)

[1] pent-1-ene acid acts as a base and accepts electrons (77)

[1] It would react poorly with an alcohol (53)

[1] Configuration

[1] Compound formed is *syn* or *trans*, doesn't matter because it takes two steps so arrangement happens. (9)

[2] Predicting Alternative Reactants for Class of Reactions

[1] The starting material could undergo similar reactions with other molecules consisting of a hydrogen bonded to a halide (70)

[1] The reaction could also take place with NaCl instead of HCl (70)

[12] Miscellanea

[1] The double bond on the reactant molecule has HCl added to its molecule to give the molecules more electrons (45)

[1] The pi bond is a source of electronegativity; H⁺ and Cl⁻ add to the C₅ that had a double bond. They don't add anywhere else (9)

[1] The carbocation is the Cl⁻ (59)

[1] HCl is used well with S_N1 reactions due to its H; S_N1 react well with O and H substrates (17)

[1] The molecule is deprotonated (36)

[1] The product molecule could be arranged as 1-chlorocyclopentane (55)



[1] A five carbon chain reacts with HCl (75)

[1] The conjugate base of HCl is Cl⁻ (42)

[1]  and HCl are the starting products (58)

[1] Chlorine is bonded to the second carbon on the product's side (60)

[1] There are no carbocations present (7)

[1] H⁺ deprotonates (4)

Creative Exercise 3

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:

A B C

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information

[44] Arene Substitution Patterns

[6] The Br and H are in the ortho position in relation to the CH₃ (5, 22, 25, 49, 72, 75)

[1] Substituents are in ortho arrangement (32)

[3] CH₃ and Br in are in ortho position (42, 55, 62)

[2] Structures above reflect ortho (38, 39)

[3] All molecules are in the ortho position. (28, 34, 78)

[1] They are in ortho position (61)

[2] These molecules are in the ortho position, which is 1,2 (4, 17)

[1] Br is in the ortho position (1:2) (48)

[1] This reaction will want to maintain an ortho or para, and is in the ortho (1)

[1] The carbocation is in ortho and para to the carbon attached to Br and H (53)

[2] This reaction would give a product that is ortho... 1,2 orientation (3, 33)

[1] Ortho (15)

[1] It's ortho (52)

[1] In A, the proton is ortho to Br (77)

[1] B, [the proton] is para, (77)

[1] C, [the proton] is in meta position (77)

[1] It is a meta (67)

[1] A, B, and C are all in the para position (14)

[1] The CH₃ and Br are meta (18)

[1] Structure A shows an ortho position of the + charge (51)

[1] Structure B shows a meta position of the positive charge (51)

[1] For A and B, the plus charge is in the meta position (74)

[1] Br and H are in the ortho stage on each molecule (30)

[1] A, B, and C are all ortho products (16)

[1] This is an ortho product (35)

[1] From "ABC" it goes: para, meta, ortho. (46)

[1] A has Br in the ortho position (76)

[1] The Br in structure B is in ortho position (12)

[1] Br and H remain in the ortho position (74)

[1] Para, bond (26)

[1] A,B,C don't like meta. (29)

[1] The position of the substituents always remain unchanged when this molecule is produced (36)

[28] Atomistic/Substituent Level

[1] They all have the same amount of electrons (61)

[2] The CH₃ is called a methyl group (4, 34)

[2] There is one methyl group attached to the molecule (60, 78)

[3] It contains 7 carbon atoms (11, 14, 49)

[1] There are 8 hydrogen atoms in this molecule (32)

[1] Halogen and methyl substituents (19)

[3] Each molecule contains a six carbon ring (11, 34, 60)

[1] They all have bromine on carbon number one (60)

[1] They are all carbocations (11)

[1] They all have carbocations (47)

[1] Each is a charged carbocation (75)

[1] The positive charge is on a tertiary carbon in C (76)

[1] The carbon attached to bromine is a secondary carbon (32)

[1] H's attached carbon is 3° (52)

[1] Br's attached carbon is 3° (52)

[1] Br has a 3° substitution (4)

[1] CH₃'s attached carbon is 2° (52)

[1] Each molecule is a tertiary structure (17)

[1] The carbocations are all on different carbons in each molecule (47)

[1] Each contains a 3° Carbon (75)

[1] Carbocation (62)

[1] The positive charge placements are due to the bromine (56)

[5] Nomenclature

[1] Product molecule is named 2-bromotoluene or 2-bromo-1-methylcyclohexane (55)

[1] The IUPAC name for A is 1-bromo-2-methylcyclohex-2,4-ene (38)

[1] The actual chemical name is 1-bromo 2-methylcyclohexene (46)

[1] The IUPAC name of this structure would be 1-bromo, 2-methyl, 2,5-cyclohexene (28)

[1] 1-methyl-6-bromo-cyclohex 1,3 ene (26)

[11] Types of Bonds

[1] It has two pi bonds, and the + occupies another pi orbital (49)

[5] Each structure has two pi bonds (14, 15, 22, 60, 75)

[1] There are four carbons with pi bonds (13)

[1] Each molecule above has 2 double bonds (34)

[1] The double bonds must alternate with single bonds (35)

[1] The double bonds are made up of a pi bond and a sigma bond (57)

[1] Electrons in pi bonds are in p orbitals (13)

[13] Classification of Structure

[1] All of the molecules have benzene rings as the parent (51)

[1] It's a benzene ring like molecule (18)

[1] It is a hexane (67)

[1] It has a cyclohexane base structure (69)

[1] The parent ring is cyclohexane (74)

[1] They all have a cyclohexane ring (10)

[1] Molecule is a cyclohexane with substituents (45)

[2] Represent alkenes (60, 75)

[1] Each molecule has 6 carbons, making it a cyclohexadiene (17)

[1] Each molecule is classified as an alkene, which is characterized by the double bond. (17)

[1] The parent chain in this molecule is a hexene ring. (36)

[1] Is an alcohol (7)

[12] Classification of Chemical Reaction

[2] The three molecules are the possible intermediates for an electrophilic substitution reaction (51, 53)

[2] This is an electrophilic substitution reaction (11, 25)

[1] In a $E_A S$, this reaction is synthesized by $Br_2/FeBr_3$ (63)

[1] This molecule could undergo $E1$ substitution reaction. (31)

[1] $SN1$ or $E1$ could be used for a reaction (29)

[1] This isn't an electrophilic substitution because the double bonds are moving (64)

[1] This is an SN_1 reaction (48)

[2] $E1$ elimination (19, 39)

[1] This molecule could go through an elimination reaction. (35)

[18] Aromaticity

[10] All of these structures are not aromatic (8, 15, 18, 28, 29, 36, 47, 62, 70, 78)

[1] None of these are aromatic products (16)

[1] This is not an aromatic ring as there are four electrons in the pi bond in each (79)

[1] It is not aromatic because there is not a pi orbital on every atom (49)

[1] These structures are not all aromatic (61)

[1] Aromatic molecule (65)

[2] These are aromatic molecules (10, 71)

[1] The molecule(s) are aromatic ($6\pi e^-$) (55)

[1] Identification of Nucleophiles/Electrophiles

[1] They are all electrophiles (11)

[15] Identification of Intermediates

[2] The three molecules are the possible intermediates for an electrophilic substitution reaction (51, 53)

[1] The three diagrams are all carbocation intermediates due to resonance (54)

[1] Three arrangements of a carbocation intermediate are shown (55)

[1] The structures are carbocation intermediates (42)

[4] A, B, and C are all intermediate resonance structures (30, 33, 65, 76)

[2] Shows the intermediates (11, 27)

[1] They are intermediates to a reaction (10)

[1] Three intermediates of a two step reaction (25)

[1] A, B, and C shows the transition state of Br being added to



(20)

[1] Structures A, B, and C are all interchangeable intermediate steps to a reaction (38)

[38] Resonance Structures

[3] Structures A, B, and C are all resonance forms (26, 38, 42)

[4] It is a resonance structure (49, 53, 57, 71)

[4] These are all forms showing different possibilities of resonance in the structure (3, 14, 28, 74)

[1] The diagram shows different resonance structures (78)

[4] A, B, and C are all intermediate resonance structures (30, 33, 65, 76)

[1] This shows a resonance structure from the charge moving around, charge is being shown that is not in one spot. (82)

[1] These are three different resonance forms for benzene derivatives (9)

[1] The charge is moved around via resonance (72)

[1] Has resonance/charge moves around ring (15)

[1] Positive charge is delocalized throughout ring (19)

[1] Shows how the (+) is spread out through resonance (11)

[1] The molecule may change from $A \rightleftharpoons B$ and $B \rightleftharpoons C$, but not $A \rightleftharpoons C$ (36)

[1] Each picture is a depiction of where the charge could be at any point in time (19)

[1] Each of the three intermediates represents a different arrangement of pi bonds (25)

[1] The resonance structures show the ability of the molecule to spread out the charge, making the molecule more stable (57)

[1] The molecules show resonance, which helps stabilize the molecule (17)

[1] A, B, and C are all the same compound with different arrangements of the + charge but the same chemical formula (79)

[1] Each one of these is a different version of the same molecule (47)

[1] The \leftrightarrow arrow is not a reaction arrow, but instead is to show different forms. (71)

[1] The electron can delocalize (18)

[1] The carbocation is moving to different carbons making it more positive than the others (45)

[1] The cation moves based on stereochemistry/resonance (69)

[1] The plus signs indicate the different resonance structures possible (4)

[1] Resonance structures allow halogens to stabilize carbocations (13)

[1] Resonance is what is stabilizing this atom by moving the positive charge around with the breaking and addition of the double bond (22)

[1] The carbon bonds rotate along with the positive charge (78)

[1] Double bonds rotate throughout the molecule (45)

[42] Directing Groups

[13] Methyl group is o, p directing (8, 9, 12, 13, 14, 25, 56, 57, 70, 72, 73, 74, 76)

[1] When CH_3 is attached to a benzene, it typically adds reactants to the ortho or para position. (20)

[6] CH_3 is an electron donating group (8, 12, 13, 32, 35, 66)

[6] CH_3 is activating group (3, 41, 56, 63, 66, 72)

[3] Br is a deactivating group (3, 9, 56)

[1] Br group is ortho-para director (14)

[1] Br is a halogen, but ortho-para directing (56)

[2] Br is electron withdrawing group, but para/ortho directing (8, 13)

[1] To form this product either the CH_3 or the Br group could have been attached first because they both favor ortho, para positions. (5)

[1] This is an ortho-directed reaction (63)

[1] Br could also have been placed in the para position. (72)

[1] This reaction will want to maintain an ortho or para, and is in the ortho (1)

[1] The bromine could have also added to this location, because activating groups are ortho-para directors. (41)



[1] It prefers the para and ortho directors. (66)

[1] Molecule has an ortho director (45)

[1] Br on the benzene prefers ortho, para (9)

[1] This is an electron donating group due to the CH_3 (1)

[3] Identification of Leaving Groups

[1] Br would be a leaving group in this reaction due to it being a stronger base (1)

[1] Br is the best leaving group for these (61)

[1] The Bromine is the best leaving group, followed by the methyl group. (46)

[12] Description of Bonding (Breaking/Forming)

[2] CH_3 was added to benzene ring first, Br second (54, 70)

[1] A, B, and C can be easily deprotonated (this is a middle step of a reaction that will lead to the molecule being deprotonated to become stable) (14)

[1] The previous step put the Br on (27)

[1] A double bond will form again to stabilize the benzene structure (9)

[1] These groups being added to the benzene ring could have been added in any order, but it makes sense to add CH_3 first, because then adding Br would be faster as CH_3 is an activating group (41)

[1] Formed by the substitution of Br into the ring (62)

[1] A negatively charged chemical could bond to the positive charge and make the benzene ring stable (82)

[1] Alkyl halides can still undergo elimination reaction if they can form stable carbocation (39)

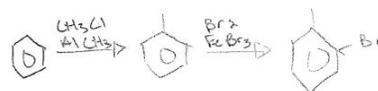
[1] Hydrogen would bond with another H to make H_2 gas or OH to make H_2O . (82)

[1] E1 elimination occurs in two steps (39)

[1] In order to make the alkene into an alkane, the double bond must be broken. (17)

[7] Reaction Schemes

[1] A possible reaction series could be (20)

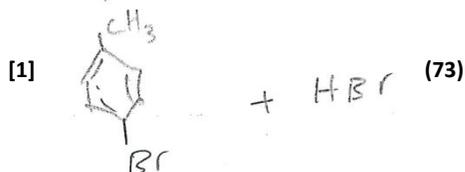
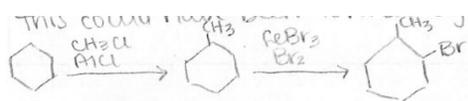


[1] If we started with benzene, the first rxn would be $\text{CH}_3\text{Cl AlCl}_3$ to add the $-\text{CH}_3$ group; second rxn would be $\text{Br}_2 \text{FeBr}_3$ so the halide joins in the ortho position. (55)

[1]  + $\text{Br}_2 \text{FeBr}_3$ ->  complete product (63)

[1]  + $\text{Br}_2 \text{FeCl}_3$ -> (73)

[1] This could have been formed by (1)

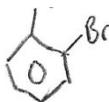


[1] Mechanism

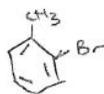
[1] E1 elimination, Breaking C-X bond to form carbocation intermediate followed by the loss of H⁺ to form alkene (39)

[9] Predicting Final Product

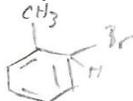
[4] The final product is (14, 48, 67, 70)



[1] The final product would be (notice placement of pi bonds) (20)



[1] The final product is (54)



[1] These are all 3 possible products of one reaction (35)

[1] Another way to draw the product would be (20)



[1] A and B are the major and intermediate products (52)

[7] Predicting Starting Material/Reagents

[2] A beginning reactant might be (16, 33)



[1] This is a depiction of the carbocation intermediates formed when bromine is being added to  via Br₂/FeBr₃ (41)

[1] CH₃ was likely (could be) added to the ring using ClCH₃ and AlCl₃ (57)

[1] Is the product where  was used as a reactant (18)

[1] Base was a benzene ring (15)

[1] If the CH₃ wasn't there, the benzene got Br from this reaction (can assume) (82)



Thermodynamics

[70] Stability

[1] Intermediate B is especially stable (33)

[1] A is least stable (77)

[8] C is the most stable (4, 21, 31, 32, 61, 69, 70, 77)

[1] C is the most stable of all. Positive charge to an E donating CH₃ (9)

[1] C is especially stable (26)

[1] C is the most stable of the three in their current state (29)

[1] If this were in a reaction problem, C would be the intermediate that is especially stable (10)

[1] B is not as stable as C due to the + charge location (79)

[16] "B" is the most stable (8, 12, 30, 38, 42, 45, 46, 48, 50, 53, 54, 63, 64, 65, 71, 76)

[1] "B" is the most stable product (16)

[1] Group "B" will be the most stable (5)

[1] Formation B would be the most reactive formation by moving the positive charge away from the cluster of groups (22)

[1] B is not a stable carbocation (47)

[9] Structure C is the least stable form (8, 28, 30, 34, 42, 46, 53, 54, 71)

[2] C is not very stable (27, 62)

[1] C is very unstable and not good to happen. (20)

[1] Structure C is the least stable product (16)

[1] Structure C would not be stable. You don't want a charge on the CH₃ (82)

[1] Structure C is bad due to the positive charge placed on carbon attached to CH₃ (3)

[1] C is least likely intermediate (65)

[1] Structure C is very unstable, due to stereogenic crowding of the alkyl group and the positive charge (51)

[2] In step C, you have a (+) next to a (+), which is BAD (30, 33)

[1] The letter C is a bad one because the (+) and the CH₃ (+) are together. (66)

[1] C is the most stable configuration because CH_3 is an activating group (41)

[1] If these were intermediates, the order would most likely be C, B, A (50)

[1] C is the most stable because the + charge is close to CH_3 (79)

[1] Configuration C is most stable because it has the + and - charges together (55)

[1] The most stable resonance form would be C due to the (+) being with the (+). (1)

[1] The orientation of "C" will not be a good group to produce and will be very unstable (5)

[1] The product above A is the most stable out of the three forms (20)

[1] A and B are the stable ones (66)

[1] Formation A would be the most stable formation of this molecule due to the electronegativity of the molecule (22)

[1] No aromatic stability (19)

[1] If iodine replaced bromine, it would increase the reactivity of the molecule. (36)

[1] The most stable form of the three would be in para with the + charge under the CH_3 , works for A, B, C (29)



[1] B is not as stable as C due to the + charge location (79)

[1] Carbocation: stability: spread out positive charge (more stable) inductive effect and hyperconjugation (39)

[1] Group "A" will be a stable group, but not the best option (5)

[1] This product would have a higher reactivity than benzene because CH_3 is a stronger activating group than bromine is a deactivating group. (41)

[1] Energy

[1] C has the highest energy (50)

[2] Reaction Rates

[1] Reaction would occur fastest with B as intermediate (65)

[1] CH_3 does react faster and is more reactive than benzene (66)

[6] Miscellanea

[1] C has a double plus charge (67)

[1] The + is rotating clockwise (67)

[1] Has stereochemistry (7)

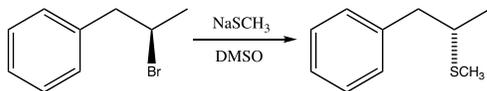
[1] They all lack three-dimensionality within this given drawing (10)

[1] The low steric hindrance makes it possible for carbocation (12)

Creative Exercise 4

Provided Prompt

Write down five **correct, distinct, and relevant** facts about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

[4] Nomenclature

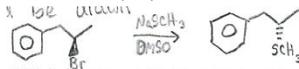
- [1] The starting material is R-2-bromo-propane attached to a cyclohexene (17)
- [1] Hex-3-ene is the main component of both (69)
- [1] The first structure is 3-bromylcyclohexane (61)
- [1] The second structure is 3-sufocyclohexane (61)

[39] Atomistic/Substituent Level

- [3] There are 9 carbons in the first molecule and 10 carbons in the second (41, 55, 78)
- [1] There are 9 carbons on the reactants side (60)
- [1] There are 9 carbons in the substrate molecule (14)
- [1] Both molecules include a carbon ring (34)
- [1] Both molecules contain a functional group (34)
- [4] SCH₃ is replacing Br (47, 58, 74, 79)
- [1] SCH₃ is substituted in place of Br (65)
- [1] The bromide is broken off and is replaced with SCH₃ (22)
- [1] Bromine was replaced with sulfur, carbon, and hydrogen atoms (33)
- [1] Br is a secondary halide (54)
- [1] There is only one tertiary carbon found in the product (11)
- [1] There is 1 tertiary carbon in each molecule (32)
- [3] There is a primary carbon present in each molecule (5, 33, 52)
- [1] They could be written as (38)

[1] The molecules can also be rewritten as (45)

[1] Could be drawn (29)



- [1] The Br is a secondary (74)
- [1] Br is in a secondary position (13)
- [1] 2° Br is substituted (62)

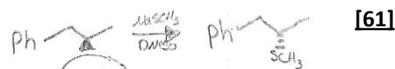
[1] The hexyclo ring doesn't change during the reaction (58)

- [1] Both molecules contain 9 carbons (34)
- [1] There are 10 hydrogen atoms per molecule (32)
- [2] Na has a negative charge (4, 8)
- [1] It is placed on a tertiary bond. (67)
- [1] There are 6 tertiary bonds (67)
- [1] There are no tertiary carbons present (50)
- [1] Benzene has chemical formula C₆H₆. (39)
- [1] The Na has a + charge (72)
- [1] The SCH₃ has a - charge (72)
- [1] Br is a halogen (75)
- [1] The Br on the original compound stands for Bromine (74)

[26] Classification of Structure

- [4] Each molecule on product and reactants contains a benzene ring (32, 56, 67, 78)
- [1] The substituents are attached to a benzene ring (71)
- [1] The base is a propyl group connected to a benzene (25)
- [2] Contains a benzene ring (18, 75)
- [1] is a benzene ring (4)
- [2] Parent ring is a benzene (60, 65)
- [1] Product contains a benzene ring (11)
- [1] The molecule that is reacting contains a benzene ring (14)
- [1] The cyclic structure on the reactant and product is a phenyl group (31)
- [1] The basic compound of this molecule is benzene (22)
- [1] Solution and product both contain benzene ring (15)
- [1] The propyl is connected to a 6-C ring. (6)
- [2] Both molecules have a phenol (Ph) group (38, 41)
- [1] Another name for this benzene ring is phenol (9)
- [1] Both contain a cyclohexane ring (10)
- [1] The parent chain is a cyclohexene molecule (36)
- [1] is called benzoic acid (79)

- [1] Has a hexyclo ring on product (58)
- [1] Has a hexyclo ring on reaction (58)

**[1] The R group of the molecule in benzene ring structure (25)****Classification of Reaction**

- [11] This is an S_N2 reaction. (1, 14, 15, 19, 22, 26, 29, 35, 41, 52, 66)
- [9] The reaction is a S_N2 substitution (5, 9, 20, 28, 30, 38, 45, 62, 70)
- [1] It is an S_N2 reaction (nucleophilic substitution) (49)
- [2] This is an S_N2 replacement reaction (27, 31)

[16] It'll do a substitution reaction. (2, 6, 11, 13, 32, 43, 47, 48, 53, 60, 63, 65, 67, 69, 75, 76)

[1] S_N2 reactions are one-step reactions (41)

[2] The reaction is a replacement reaction (16, 25)

[1] It is an exothermic reaction (36)

[1] A substitution reaction occurs between Br and SCH_3 (36)

[1] Electrophilic substitution reactions (like this) are used for alkyl halides (51)

[1] This is an electrophilic substitution reaction (51)

[4] This is an S_N1 reaction (16, 55, 56, 60)

[1] This is a S_N1 reaction (substitution) that involves an electrophile. (50)

[1] This can be done by S_N1 or E1 reaction (12)

[1] This is an E1 reaction (2 step) (46)

[1] This is not an equilibrium reaction (38)

[1] This reaction would also be an E_2 reaction as it is a one-step and the Br and SCH_3 are secondary (1)

[1] At Br and SCH_3 a addition reaction could be done (29)

[4] The reaction is a substitution reaction (20, 28, 45, 62)

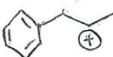
[1] This is not an elimination reaction (74)

[4] Identification of Intermediates

[1] No intermediate carbocation is formed (66)

[1] No carbocation is formed because it is not S_N1 reaction (49)

[1] $NaSCH_3$, DMSO are the intermediates to this reaction (10)

[1] An intermediate might be  (16)

[11] Identification of Nucleophiles/Electrophiles

[1] The SCH_3^- is the nucleophile. (35)

[1] Na^+ is the electrophile. (35)

[3] Br is acting as the nucleophile (28, 47, 48)

[1] Br underwent nucleophilic attack (10)

[1] Na^+ is a nucleophile looking for Br^- (49)

[3] SCH_3 is acting as the electrophile (28, 48, 70)

[1] $NaSCH_3$ is the electrophile (50)

[12] Types of Bonds

[2] Both molecules have 3 double bonds (34, 41)

[1] This structure contains three double bonds (pi bond) (39) 

[1] There are 3 pi bonds in the substrate molecule (14)

[2] There is 6 sp^2 hybridized carbons in each molecule (5, 34)

[1] The reactants contains 6 sp^2 hybridized carbons. (35)



have a total of 12 sp^2 hybridized carbons (20)

[1] There are 6 double bonds in the benzene ring (4)

[1] Double bond contains one sigma and pi bond (39)

[1] Each benzene ring is sp^2 hybridized for each p orbital (67)

[1] The double bonds in the cyclohexene tells us that the molecule contains sp^2 hybridization (17)

[20] Description of Bonding (Breaking/Forming)

[2] This is a one step reaction (48, 66)

[1] SCH_3 bonds to  the same time Br

leaves so it is into the page (9)

[1] It is a one step reaction with Br leaving and SCH_3 coming at the same time (49)

[1] The DMSO helps remove the Br (72)

[1] Br attacks Na (47)

[2] This is a two step reaction (71, 79)

[1] Metal (Na) is used to remove Br from reactant (65)

[1] Na and DMSO will remove the bromine molecule (56)

[1] Na^+ bonds with Br^- to take it off the carbon. (35)

[1] Na breaks off Br from the molecule to form NaBr (22)

[1] Na reacts with Br to remove it from its position on the 2 carbon (16)

[1] The sodium is what takes the bromine away (61)

[1] Na from $NaSCH_3$ knocks off the Br. (4)

[1] After Na knocks off Br, SCH_3 is added in its place (4)

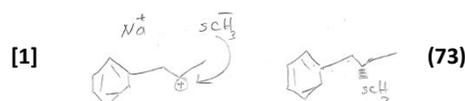
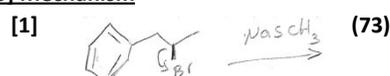
[1] During the reaction the Na^+ from $NaSCH_3$ will take Br off and replace with SCH_3 (29)

[1] When the Br leaves, there is a carbocation for the SCH_3 to bond to (13)

[1] A hydrogen anti to the bromine is removed (8)

[1] Na^+ masks the negative charge (48)

[3] Mechanism



[21] Identification of Leaving Groups

[9] The bromine is acting as a leaving group (10, 12, 14, 25, 43, 49, 52, 61, 75)

[6] Br served as a good leaving group (3, 8, 56, 57, 64, 70)

[1] Br is a good leaving weak group (66)

[1] Br is a good leaving group, which allows for the SCH_3 to be substituted (1)

[1] The leaving group is tertiary (12)

[1] SCH_3 attacks Br because Br is a good leaving group (64)

[1] The leaving group is NaBr (76)

[1] Bromine is one of the best leaving groups (61)

[10] Identification of by-products

[8] A byproduct is NaBr (8, 9, 14, 22, 25, 32, 54, 70)

[1] During the reaction Br splits from the molecule and forms an ionic bond with Na (31)

[1] The Br bonds to the Na after leaving (15)

[17] Aromaticity

[3] Both of these molecules are aromatic (30, 62, 70)

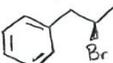
[4] Both molecules contain an aromatic ring (2, 53, 60, 76)

[2] Both product and reactant have an aromatic benzene ring (29, 55)

[1] The ring is aromatic (15)

[2] The benzene rings are aromatic (46, 71)

[1] Aromatic ring is unsaturated hydrocarbons. (39)

[1]  is aromatic (57)

[1] Neither compound is aromatic (8)

[1] Each benzene ring follows the equation $4n + 2$ for number of electrons it contains (67)

[1] Aromatic (43)

[2] Resonance Structures

[1] Both have multiple resonance forms (53)

[1] The ring has resonance (54)

[10] Stability

[1] The result is more stable (69)

[1] The molecule on the right is the most stable (2)

[2] The product is more stable than the reactants (30, 50)

[1] The molecule becomes more stable after the reaction (46)

[1] $-SCH_3$ is more reactive than $-Br$ (55)

[1] The rings shown are likely in chair formations, which are more stable than boat formations (57)

[1] It is a more stable molecule than any alkane (36)

[1] The product is less stable than the starting molecule (28)

[1] Both are relatively stable (53)

[5] Reaction Rate

[1] DMSO is a good solvent for S_N2 reactions (faster rate) (51)

[1] $NaSCH_3$ is a proton withdrawing group, and would make for a faster reaction time (1)

[1] This reaction will be slower than a normal benzene ring (63)

[1] The time it would take to react decreased (33)

[1] CH_3 and OH react faster than benzene in electrophilic substitution reaction. (39)

[1] Directing Groups

[1] $-Br$ is a weak deactivating group (63)

[17] Properties

[1] $NaSCH_3$ and DMSO are reagents (74)

[1] A aprotic solvent is used to help the reaction proceed (9)

[1] DMSO is an aprotic, and typically used for S_N2 reactions. (1)

[5] DMSO is a catalyst. (2, 6, 19, 27, 54)

[1] DMSO acts as a catalyst to speed up the reaction (17)

[1] The product is an acid (18)

[1] The one of the left is more acidic (53)

[1] DMSO is a common catalyst in benzene reactions (18)

[1] DMSO is a constitutional isomer (40)

[1] DMSO is acting as an enzyme (47)

[1] Catalyst – $NaSCH_3$ DMSO (43)

[1] The solvents is protic (12)

[1] Nucleotide – SCH_3 (43)

[27] Stereochemistry

[1] It is a chiral molecule (67)

[1] There is an inversion of configuration (49)

[1] It has one chiral carbon (63)

[4] One stereogenic carbon on each molecule in product and reactant (2, 52, 67, 78)

[1] One stereogenic carbon (19)

[1] Product contains a stereogenic carbon (11)

[2] The reaction takes place on a stereogenic carbon (25, 50)

[1] An inversion happened (66)

[1] Orientation of substituent group reverses (75)

[1] The orientation of the functional group is changed between the products and reactants (36)

[1] The product side, SCH_3 is in the down position which is drawn with  (84)

[2] The Br is pointing off the paper towards us (55, 79)

[1] Br and SCH₃ differ within 3-dimensionality within the molecule (10)

[2] Br is coming towards us while SCH₃ is going away. (6, 52)

[1] Br is coming out toward you (81)

[1] When this reaction happens, it goes from Br towards you to SCH₃ away from you (22)

[2] The SCH₃ is facing from us on the stereogenic carbon (55, 79)

[1] SCH₃ is going behind or away from you (81)

[1] The reactant side, Br is in the up position which is drawn with  (84)

[1] Has stereochemistry (7)

[50] Configuration

[16] In the first molecule the Br is in the R configuration. (1, 5, 13, 17, 18, 19, 27, 30, 33, 38, 40, 45, 62, 63, 71, 76)

[1] The chiral carbon on the reactant is R (31)

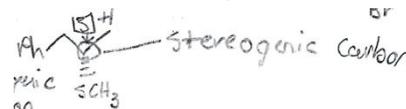
[1]  (50)

[1] The solution is a R configuration (15)

[1] The stereogenic carbon on the reactant side is right-handed (57)

[14] In the second molecule the SCH₃ is in the S configuration (1, 5, 11, 13, 17, 19, 27, 30, 33, 38, 45, 62, 63, 76)

[1] The chiral carbon on the product is S (31)

[1]  (50)

[1] The stereogenic carbon on the product side is left-handed (57)

[5] The SCH₃ is R-configuration (18, 40, 71, 72, 84)

[2] The Br is S-configuration (72, 84)

[1] Compound begins as cis and ends up in trans (33)

[1] Br and SCH₃ are trans in relation to each other (65)

[1] -SCH₃ adds trans to the original -Br substituent (51)

[1] The two molecules are trans of each other since Br is in front and SCH₃ is in the back (17)

[1] The SCH₃ attached anti to Br (54)

[1] S configuration. (67)

[1] Reaction Energy Diagrams

[1] The graph would look like  (58)

[11] Miscellanea

[1] The reaction forces the Br and SCH₃ to flip resonance structures (46)

[1] This reaction cannot go in reverse because the bromine is too weak (46)

[1] DMSO is used to make the leaving group better (20)

[1] NaSCH₃ is a bulky base. That's why DMSO is needed to make the reaction start (51)

[1] The benzene ring makes it easier for a reaction to take place because of its aromaticity (12)

[1] If you cross out Na and make SCH₃ negative you can put it where Br is if its positive (84)

[1] DMSO caused Br to face away, go from wedge to dash (3)

[1] SN₂ reactions prefer polar protic solvents such as NaSCH₃ (20)

[1] This is an easily reversible reaction (69)

[1] Br wants to gain an electron. (6)

[1] This changes the structure and composition (6)

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3 The data supporting this article have been included as part of the Supplementary
4 Information.
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