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Harnessing the Power of Virtual Reality for Organic Chemistry Education

A thesis presented in Candidacy for Departmental Honors in Chemistry

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from

The College of William and Mary in Virginia

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May 8th, 2024

Accepted for HONORS

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Abstract

Understanding organic chemistry concepts heavily relies on visualization of the geometry of molecules and spatial arrangement of molecules during mechanisms. 2D textbook depictions have their limitations in visualizing the three-dimensionality of organic chemistry. Student learning outcomes could be greatly improved from 3D visualizations of these topics. This project explores the potential of an emerging technology, Virtual Reality (VR), being incorporated as a teaching resource for organic chemistry.

This paper discusses two trials for evaluating the potential of VR as a teaching resource for organic chemistry in select topics of the Diels-Alder reaction and R/S configurations and stereoisomers. The Diels-Alder reaction is a fundamental Nobel-Prize winning reaction taught in Organic Chemistry II. Experience has proven that students often struggle to visualize the transition state of this reaction and to predict the correct organic products, both in terms of regiochemistry and stereochemistry. R/S configurations and stereoisomers is a topic taught in Organic Chemistry I in which students often struggle to visualize 3D molecules to correctly assign the configuration of chirality centers and further determine the relationship between stereoisomers. Hence, we chose to develop VR organic chemistry learning exercises for these topics, which might enhance students' understanding of the reaction compared to traditional teaching by taking advantage of the immersive and interactive experiences created by VR. This paper shows that VR tutorials have comparable student learning outcomes to traditional learning and students enjoyed learning with VR more than in a traditional classroom setting. The ethnicity or gender identity of the student did not seem to affect student benefits from the VR experience, which shows the potential of VR as an equitable

teaching resource for organic chemistry. The methodology of VR development is also discussed in this paper as reference for future novice VR developers.

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Chapter 1 Introduction to Virtual Reality and its Utility in Chemistry Education

1.1 Introduction to Virtual Reality (VR)

Virtual Reality (VR) is an emerging technology that can simulate an immersive environment within which the user can exist and interact with the simulated objects, effectively mimicking experiences in reality¹. These simulations are often presented to the users on multiple screens around the user or on a wearable display². The multiple screens display provides users a non-immersive VR experience, while a head-mounted display (HMD), such as the Meta Quest 2, provides users an immersive VR experience². In an immersive VR experience, users are presented with a 360-degree virtual environment around them, and the head and hand movements of the user are reflected in the virtual environment with the help of movement tracking sensors in the HMD and the controllers². As VR developers continue to be innovative and VR consoles become more accessible to the public, more sectors have been incorporating VR, notably in gaming, health care, and education¹.



Figure 1.1. Meta Quest 2 Headset (middle) and Controllers (left and right)³.

1.2 Potential of VR in Chemistry Education

While traditional learning is the most abundant teaching method, it has limitations. One criticism is that learners find traditional methods to be unengaging and taught content often have variability between instructors due to different emphasis on topics or pacing of the class¹. Reviewing instances where VR was used in education, Gunawan's group found that every discipline that has existing knowledge could take advantage of using VR to teach users new concepts or reinforce concepts¹. In education, the use of VR as a teaching aid has potential to increase participation and opportunities as well as enhance learning. This is made possible by the fact that VR mimics real world experiences, so the skills students learn in the VR environment is transferable to the real world¹. VR can further help increase attention levels of students as the HMD can help in eliminating visual and auditory distractions from the real world². Some advantages of VR learning include being engaging through its audiovisual experience, increasing creative problem-solving skills for the students, and avoiding potential negative consequences from choices made during the learning process¹. Gunawan's group also found that many study results seem to support the idea that VR learning is more effective than traditional learning¹. The use of VR especially increased during the COVID-19 pandemic as a novel method of delivering asynchronous lectures, and VR was reported to be more engaging to students than watching videos².

VR learning, however, is not without flaws. One of the limitations of VR learning is that since VR content has to be developed beforehand, the range of questions that can be answered within the VR experience is limited to what the developers are able to predict as the students' questions². Therefore, Hamad's group concluded that VR

cannot replace traditional learning due to its inability to adapt to various real-time questions posed by the students². Another limitation of VR is the lack of standardization of VR often leading to difficulty in transferring applications between different device types. Moreover, VR development requires decently powerful computers which are not accessible to all. Finally, the physical strain on the eyes and neck due to the HMDs can cause "cybersickness", which is a type of motion sickness induced by VR². Cybersickness is most likely due to the slight lag in the HMD's virtual world display compared to the real-world movements².

Despite its limitations, VR is steadily establishing its use in science, technology, engineering, and mathematics (STEM) education, as it can promote active learning as opposed to the more often passive traditional learning⁴. Students can also safely experience diverse environments in a short time, and even experience environments that would be impossible to explore in the real world². VR can also help bypass safety concerns. For example, in a chemistry lab learning context some students are inadequately prepared to be in a real-life laboratory with toxic chemicals and potentially dangerous instruments⁵. The limitation that the VR content must be developed beforehand is still an important concern in STEM education. Many experimental results are unpredictable, so it is implausible to foresee all the possible outcomes of the experiments in order to develop VR that is comprehensive⁵.

Viitaharju's research group delineated the potential advantages and limitations of using VR as a chemistry laboratory supplement. In this study first-year chemical engineering students at Aalto University were tasked with virtual laboratories before their real-life laboratory exercises on flame atomic absorption spectroscopy (AAS) or UV-Vis spectrophotometry⁶. Student feedback revealed that while many students thought the videos of every step of the lab being carried out was interesting, the videos could become too repetitive and were slow-paced⁶. On the other hand, students also reported that the interactive questions in the virtual laboratory were interesting, while the instructions in PDF format were reported as boring⁶. Many students agreed that they thought that the real-life laboratory exercise was easier, and they felt more comfortable in the real-life laboratory after completing virtual laboratory⁶. However, most students also reported that they thought the real-life laboratory after completing virtual laboratory⁶. However, most students also reported that they thought the real-life laboratory was more interesting than the virtual laboratory⁶. This suggests that VR has potential as a supplemental learning tool in chemistry education rather than a replacement⁶.

1.3 State of the Art

There are numerous instances where VR was used to aid in educating users about a chemical process, mechanism, or proper protocol in a laboratory setting. Lu's group developed the Virtual Reality Remote Education for Experimental Chemistry system that teaches users how to synthesize gold nanocrystals to address the lack of resources to remotely continue experimental chemistry education in times such as COVID-19⁵. Broyer developed an immersive VR tutorial on glove hygiene in a chemical laboratory to help first year undergraduate chemistry laboratory students feel more comfortable about entering their first chemistry laboratory and to promote appropriate glove use in the laboratory⁷, and Dr. Emmanuel Echeverri-Jimenez developed a VR tutorial for the Diels-Alder mechanism in 2022⁸. During the COVID-19 pandemic, many institutions including the William & Mary Chemistry Department incorporated the Virtual Reality Organic Chemistry Labs that were previously developed by North Carolina State into the remote Organic Chemistry I lab. North Carolina State generously offered all of its developed Organic Chemistry VR laboratory content to other institutions free of charge, aiding them in navigating the abrupt shift to online learning prompted by the pandemic⁹.

NC State's VR Organic Chemistry Labs include virtual exercises on various topics from laboratory techniques and lectures, such as Thin Layer Chromatography (TLC), Extraction, and SN2 Reactions of Alkyl Halides⁹. There are two major modes of delivery for these labs: on a computer or on a mobile device⁹. On a computer, students would navigate through the user interface of the tutorials and view the 360-degree laboratory environment using a mouse or keyboard⁹. On a mobile device, students could choose the Google Cardboard option to place their phone into the Google Cardboard, where they can move their head to view the 360-degree environment, just like in a Meta Quest headset⁹. Unfortunately, this option was not available for investigation as the application used to launch the VR lab was designed for an older version of Android. In the computer delivery of the 360-degree laboratory environment, there is a teaching assistant (TA) who guides students through the exercise by reading aloud the instructions on the user interface, and students can navigate through the exercise⁹. While the experiment is performed, students can observe the hands of the TA in the video performing the steps of the experiment while the directions are read by the TA as a narration⁹. While it was helpful to watch and learn how the experiments are conducted, there are minimal interactable components. Occasionally, buttons can be pressed to prompt an action or predictions for outcomes can be selected on the user interface, but students don't have the opportunity to practice going through the motions

of the experiment themselves. It is important to note that NC State intentionally chose a diverse group of TAs to be featured in their VR labs in an effort to promote diversity, equity and inclusion.

We took the NC State's VR Organic Chemistry Labs as an inspiration and looked for possible areas of improvement. One potential area of improvement was the use of adaptive release, where specific material is released based on meeting one or more criteria. NC State's VR Organic Chemistry labs were formatted with short, replayable 360 video segments that students could look around in, with occasional questions that check for understanding⁹. However, there were no features in the VR labs that prevented students from skipping to the end of the video clip, or neglecting to answer the questions that check for understanding. The lack of features that control the release of subsequent content in an asynchronous environment such as a VR lab has the potential for exploitation by students as they can complete the exercises without much understanding or engaging with the material. With the use of adaptive release, we can control if the subsequent topic should be presented to the user based on whether the student completes the previous task that is necessary for understanding the next segment's topics. We acknowledge that even with adaptive release it is still possible for students to mindlessly navigate to the end of the tutorial by randomly clicking all the possible answers, however they would still have to be exposed to the correct answer and the feedback before they can move on to the next topic.

While developing VR tutorials for this research, we hoped to implement adaptive release and increase the interactiveness of the VR tutorials compared to NC State's VR Organic Chemistry Labs because we wanted to take full advantage of the immersive

and interactive nature of a VR environment. This is by no means a critique of the NC State's VR labs; in fact, we view them as a pioneering development that we hope to build upon.

Chapter 2 - Application in Organic Chemistry 2

2.1 The Diels-Alder Reaction

The Diels-Alder reaction is a cycloaddition between an alkene or an alkyne and a conjugated diene. The alkene (contains a double bond) or alkyne (contains a triple bond) is called a dienophile, and a conjugated diene is a molecule with two double bonds that are separated by exactly one single bond. This reaction is a cycloaddition because its products are cyclic. The reaction mechanism results in two new σ bonds and one new π bond forming, and three π bonds breaking, as shown in **Scheme 2.1**.



Scheme 2.1. A Simple Diels-Alder Reaction Mechanism. Two new σ bonds and one new π bond are formed and three π bonds are broken.

The stereochemistry of the product depends on the stereochemistry of the dienophile and the diene. A case where the stereochemistry of the product depends solely on the stereochemistry of the dienophile is shown in **Scheme 2.2.** A *cis* dienophile results in a *syn* product, whereas a *trans* dienophile results in an *anti* product.



Scheme 2.2. A Diels-Alder Reaction with Substituted Dienophile.

A case where the stereochemistry of the product depends solely on the stereochemistry of the diene is shown in **Scheme 2.3.** Substituents that pointing toward the "outside" on the diene (ethyl group in **Scheme 2.3**) and substituents that are pointing toward the "inside" of the diene (methyl group in **Scheme 2.3**) end up *anti* to each other in the product. Substituents that are both pointing to the "outside" of the diene or substituents that are both pointing to the "inside" of the diene of the diene end up *syn* to each other in the product.



Scheme 2.3. A Diels-Alder Reaction with Substituted Diene.

A case where substituents on both the dienophile and the diene contribute to stereochemistry is shown in **Scheme 2.4.** This case can lead to *endo-* and *exo-* products, which are diastereomers. In the major *endo-* products the "outside" groups on the diene end up in a *syn* conformation with respect to the electron withdrawing groups on the dienophile, whereas in the minor *exo-* products the "outside" groups on the dienophile, whereas in the minor *exo-* products the "outside" groups on the dienophile. **Scheme 2.4** also shows that the Diels-Alder reaction can form bicyclic products if the diene is cyclic. A bicyclic product would also form if the dienophile were cyclic.



Scheme 2.4. A Diels-Alder Reaction with Substituents on Dienophile and Diene.

2.2 Diels-Alder Tutorial

From the Organic Chemistry II curriculum, we selected the Diels-Alder reaction for development of a VR tutorial. The products of Diels-Alder are cyclic, which would be excellent to view with 3D models in VR. In some cases, the Diels-Alder reaction produces major endo- and minor exo- products, which are diastereomers and would be great models to compare side-by-side in VR. While designing the VR tutorial, we initially aimed to include both the stereochemistry and regiochemistry of the Diels-Alder reaction arising from different starting diene and dienophile reactants, but due to the limited time we had in developing and the difficulties in estimating the duration of the VR tutorial, we ended up developing a tutorial that focused primarily on the stereochemistry of the Diels-Alder reaction.

Features in the Diels-Alder tutorial include presentation of topics on a user interface (UI), interactive molecules and chemical reactions, and adaptive release. The tutorial curriculum was adapted from the contents of Master Organic Chemistry, summarizing the basic Diels-Alder reaction scheme and how to determine the stereochemistry of the Diels-Alder products. The layout of the topics was as follows: introduction of the Diels-Alder reaction with the reaction mechanism, structural requirements for the diene for a Diels-Alder reaction to occur, and examples of the Diels-Alder reaction. The examples of the Diels-Alder reaction were presented in increasing complexity. Initially, the stereochemical outcome of the reaction was solely dependent on the substituents of the dienophile or only on the substituents of the diene. However eventually the user is presented with complex examples where the relative stereochemistry between the diene and the dienophile comes into play and leads to the major endo- and the minor exo- products that arise from a reaction of both a substituted diene and a substituted dienophile.

The interactive feature of combining the reactants to create the product was included in this tutorial. Students could grab a diene and a dienophile together and bring them within a certain distance and they would then be presented with the product of the reaction. We wanted to also implement an undo reaction feature, where students would be able to perform the Diels-Alder reaction on a slide and click a button on the UI to reset the reaction back to its reactants. Unfortunately, we were unable to implement this feature due to time limitations.

Adaptive release was also implemented, so that students would only be able to continue in the tutorial after they have interacted with the reactant molecules to make the product molecule. Although we were able to implement adaptive release on most of the tutorial, there were instances where students were presented with two reactions to explore on one slide, for which we were unable to find a method to track if students actually explored both reactions as intended. Due to the time-consuming development, the adaptive release was not implemented on this type of reaction slide.

2.3 Diels-Alder Tutorial Data

Participants

Participants were volunteers (N = 24, 79.2% female) from 190 students enrolled in Professor Dana Lashley's CHEM 207 - Organic Chemistry II for Life Sciences sections in Fall 2023. Trials were advertised as an optional help session, which would provide an extra opportunity to engage with the Diels-Alder reaction covered in class. Various one-hour sessions were available for students to sign up on December $6^{th}-7^{th}$ and students were randomly assigned to either the VR learning group (N = 12) or the traditional learning group (N = 12).

Measures

We conducted a pre-survey and a post-survey with a questionnaire developed with Qualtrics. In the pre-survey, we collected demographic data of the students' major, race and ethnicity, gender identity, international student status, and neurodiversity status.

We also measured the comfort level of their understanding of the Diels-Alder reaction prior to the help session on a scale of 1-7, 1 being extremely uncomfortable and 7 being extremely comfortable.

In the post-survey, we asked what learning group the student was assigned to and whether they have prior experience in using VR. We measured their enjoyment level during the help session on a scale of 1-7, 1 being extremely unenjoyable and 7 being extremely enjoyable. We also measured the comfort level of their understanding of the Diels-Alder reaction after the help session on a scale of 1-7, 1 being extremely uncomfortable and 7 being extremely comfortable. Students also answered two multiple choice questions on predicting the major product of Diels-Alder reactions as part of the post-survey. Finally, students were presented with one free response question on predicting the product of a Diels-Alder reaction timed for three minutes to simulate onpaper exam conditions.

Procedure

At the beginning of each hour session, the residing investigator (Jungmin Shin) informed students on the purpose of this study, any health risks associated with the study, what data would be collected throughout the session, and that the participation in the study was voluntary. The investigator obtained signatures on the consent form from students who agreed to the above terms. Students were instructed to the Qualtrics link to answer the first page of the link to complete the pre-survey questions and set the survey aside for after the tutorial.

After the pre-survey, students in the VR learning group were administered the WM Diels-Alder Tutorial 2024 developed with the Unity game engine for the Meta Quest 2 headset. Students in the VR learning group were directed to navigate through the VR tutorial at their own pace. Students in the traditional learning group were given handouts with the same content as in the VR tutorial. For the traditional learning group, diagrams were drawn out on a white board to supplement the verbal explanations of the investigator and students were asked questions throughout the lecture to check their understanding of the content being presented and to keep them engaged in the lecture.

After the tutorial, students were directed to return to the Qualtrics link to complete the post-survey questions and submit the Qualtrics link. For the two multiple choice questions embedded into the Qualtrics survey, students were also provided with the paper version of the questions so that they could see the question better and have the option of solving the problems with paper and pencil. After the surveys were submitted, the investigator went over the two multiple choice questions, and students were asked to complete the 3-minute on-paper exam simulation.

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Data Analytic Plan

Paired samples t-tests were conducted to determine if there was a difference in comfort levels regarding the Diels-Alder reaction before and after the tutorial for the combined group of students from both the VR learning and traditional learning groups, the VR learning group, and the traditional learning group.

Independent samples t-tests were conducted to determine if there was a difference in enjoyment levels during the Diels-Alder tutorial as well as a difference in average comfort level score improvement before and after the tutorial between the VR learning group and the traditional learning group.

Factorial Analysis of Variance (Factorial ANOVA) were conducted to determine if there was a difference in enjoyment levels during the Diels-Alder tutorial as well as the difference in magnitude of comfort level changes before and after the tutorial for students of different ethnic groups or gender identity groups in VR learning group or traditional learning group.

2.4 Diels-Alder Tutorial Data Analysis

Paired samples t-tests revealed statistically significant differences in the comfort levels of the combined group of students from both the VR learning and traditional learning groups. Student reported comfort levels were higher after the tutorial (M = 6.042, SD = 0.624) than comfort levels before the tutorial (M = 5.000, SD = 1.022), t(23) = -5.108, p < 0.05, two tailed test, d = -1.043. Paired samples t-tests also revealed statistically significant differences in the comfort levels of students in the VR learning group. The comfort levels of students in the VR group after the tutorial were higher (M = 6.000, SD = 0.739) than comfort levels before the tutorial (M = 5.000, SD = 0.603), t(11) = -5.745, p < 0.05, two tailed test, d = -1.658. Paired samples t-tests further revealed statistically significant differences in the comfort levels of students in the traditional learning group. The comfort levels of students in the traditional learning group after the tutorial was higher (M = 6.083, SD = 0.515) than comfort levels before the tutorial (M = 5.00, SD = 1.348), t(11) = -2.862, p < 0.05, two tailed test, d = -0.826. We concluded that students in general found the tutorials helped in their understanding of the Diels-Alder tutorial, regardless of the tutorial mode. We also concluded that the students in the VR group and traditional learning group found the respective tutorial modes helped them in understanding the Diels-Alder reaction. Data is summarized in **Table 2.1**.

	Mean	Std. Dev.	Mean	Std. Dev.	Calculated t-
	Before	Before	After	After	value
Combined Group	5.000	1.022	6.042	0.624	-5.108*
VR Learning	5.000	0.603	6.000	0.739	-5.745*
Group					
Traditional	5.000	1.348	6.083	0.515	-2.862*
Learning Group					

Table 2.1. Comfort Levels Before and After the Diels-Alder Tutorial. Statistically significant t-values are noted with *, $\alpha = 0.05$.

Independent samples t-tests revealed statistically significant differences in the reported enjoyment level during the tutorial between the VR learning group or the traditional learning group. Students in the VR group reported higher enjoyment levels during the tutorial (M = 6.083, SD = 1.165) than students in the traditional learning group (M = 4.333, SD = 1.435), t(22) = -3.280, p < 0.05, two-tailed test, d = -1.339. Independent samples t-test revealed no statistically significant differences in the average comfort level score improvement before and after the tutorial between the VR learning group and the traditional learning group. There was no difference in the

average comfort level score improvement between before and after the tutorial for students in the VR learning group (M = 1.000, SD = 0.603) than students in the traditional learning group (M = 1.083, SD = 1.311), t(22) = 0.200, p > 0.05, two-tailed test. We concluded that in general, the students in the VR learning group reported that they enjoyed the tutorial more than the students in the traditional learning group. We were unable to conclude if there were any differences between the VR learning group and the traditional learning group in how much comfort levels increased before and after the tutorial. Data is summarized in **Table 2.2**.

	VR Mean	VR Std. Dev.	Traditional	Traditional	Calculated
			Mean	Std. Dev.	t-value
Enjoyment	6.083	1.165	4.333	1.435	-3.280*
Average	1.000	0.603	1.083	1.311	0.200
Comfort					
Level					
Improvement					

Table 2.2. Enjoyment and Average Comfort Level Improvement in Diels-Alder.

Factorial ANOVA revealed a statistically significant difference in the enjoyment levels during the tutorial for students in different learning groups, but no significant difference for students of different ethnicities. The 2x3 ANOVA revealed no significant main effects of ethnicity [F(2, 18) = 0.164, p > 0.05], but a significant main effect of learning group [F(1, 18) = 4.655, p < 0.05], but no significant interaction [F(2, 18) = 0.05], but

0.391, p > 0.05]. Data is summarized in **Table 2.3.**

Learning Group	European Non-European Mixed Ethnicity		Row Means	
	White	White	-	
Traditional	4.125	5.000	4.000	4.375
VR	6.250	6.000	6.000	6.083*
Column Means	5.188	5.500	5.000	

Table 2.3. Enjoyment Levels in Diels-Alder by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, $\alpha = 0.05$.

Factorial ANOVA also revealed no significant difference in the improvement of comfort levels after the tutorial for students of different ethnicities experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of ethnicity [F(2, 18) = 0.301, p > 0.05], no significant main effect of learning group [F(1, 18) = 0.086, p > 0.05], and no significant interaction [F(2, 18) = 0.301, p > 0.05]. Data is summarized in

Table 2.4.

Learning Group	European	Non-European	Mixed Ethnicity	Row Means
	White	White	-	
Traditional	1.125	1.333	0.000	0.819
VR	1.000	1.000	1.000	1.000
Column Means	1.063	1.167	0.500	

Table 2.4. Average Comfort Improvement in Diels-Alder by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in enjoyment levels during the tutorial for students of different gender experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of gender [F(2, 19) = 0.086, p > 0.05], no significant main effect of learning group [F(1, 19) = 2.701, p > 0.05], and no significant interaction [F(1, 19) = 0.961, p > 0.05]. Data is summarized in **Table 2.5**.

Learning Group	Female Male Prefer not to			Row Means
			answer	
Traditional	4.222	5.000	4.000	4.407
VR	6.200	5.500	Not Observed	5.850
Column Means	5.211	5.250	4.000	

Table 2.5. Enjoyment Levels in Diels-Alder by Gender and Learning Group. Statistically significant differences in mean are noted with *, $\alpha = 0.05$.

Factorial ANOVA also revealed no significant difference in the improvement of

comfort levels after the tutorial for students of different genders experiencing either

tutorial mode. The 2x3 ANOVA revealed no significant main effect of gender [F(2, 19) =

0.266, p > 0.05], no significant main effect of learning group [F(1, 19) = 0.470, p > 0.05], and no significant interaction [F(1, 19) = 1.107, p > 0.05]. Data is summarized in **Table 2.6.**

	Gender Identity			
Learning Group	Female	Male	Prefer not to	Row Means
			answer	
Traditional	0.889	1.500	2.000	1.463
VR	1.100	0.500	Not Observed	0.800
Column Means	0.994	1.000	2.000	

Table 2.6. Average Comfort Improvement in Diels-Alder by Gender and Learning Group. Statistically significant differences in mean are noted with *, $\alpha = 0.05$

We concluded that the ethnicity or gender of the student seems to not have an effect on how much the students enjoy VR or traditional learning nor does ethnicity or gender have an effect on how much more comfortable they feel about the content after VR or traditional instruction.

Content Performance

We also kept records of content performance with the check for understanding questions and the on-paper exam simulations. Check for understanding question 1 (**Scheme 2.5**) had an overall correct response rate of 0.958 (23/24), the VR learning group had a correct response rate of 0.917 (11/12), and the traditional learning group had a correct response rate of 1.000 (12/12).

Q1. Predict the major product of the following reaction (Choose one):



Scheme 2.5. Multiple-Choice Check for Understanding Question 1 for Diels-Alder. Choice 2 is the correct answer.

Check for understanding question 2 (**Scheme 2.6**) had an overall correct response rate of 0.875 (21/24), the VR learning group had a correct response rate of 0.750 (9/12), and the traditional learning group had a correct response rate of 1.000 (12/12).



Q2. Predict the major product of the following reaction (Choose one):

Scheme 2.6. Multiple-Choice Check for Understanding Question 2 for Diels-Alder. Choice 5 is the correct answer.
The on-paper exam simulation (**Scheme 2.7**) had an overall correct response rate of 0.458 (11/24), the VR learning group had a correct response rate of 0.500 (6/12), and the traditional learning group had a correct response rate of 0.417 (5/12). We were unable to conclude if VR learning had better learning outcomes than traditional learning.

Predict the product of the following reaction:



Group (Circle one): VR or Traditional Classroom

Scheme 2.7. Free-Response On-Paper Exam Simulation Question for Diels-Alder.

	Overall	VR	Traditional
Question 1	0.958	0.917	1.000
Question 2	0.875	0.750	1.000
Exam Simulation	0.458	0.500	0.417

Data on content performance for Diels-Alder is summarized in Table 2.7.

Table 2.7. Correct Response Rates for Content Performance in Diels-Alder.

2.5 Possible Sources of Error for Diels-Alder Tutorial

Data collection was conducted from December 6th-7th, 2023, which was after the Diels-Alder reaction was formally tested on an exam, and the final exam for the course was less than a week away. It is possible that student performances on the check for understanding questions did not have a statistically significant difference between the

VR learning group and traditional learning group because the Diels-Alder reaction was fresh in the students' minds and students could have been regularly reviewing the reaction in preparation for the final exam to adequately answer the questions. It is also possible that the questions were too easy, as the multiple-choice questions had 8 possible choices, some of which were chemically nonsensical and could be easily eliminated as a possible answer. It is also possible that the content questions were administered too soon after the tutorials to adequately measure if the students were better able to internalize the Diels-Alder reaction and retain the content over time.

Chapter 3 - Application in Organic Chemistry 1

3.1 R/S Configurations and Stereoisomers Background

Molecules that are non-superimposable mirror images with respect to one another are called enantiomers. Molecules that exhibit biological properties by binding to a receptor are called "biologically active" and are often of interest in drug development. The biological properties of two enantiomers can be drastically different. Often, only one of the enantiomers is biologically active while the other enantiomer is not active. This also applies to natural products, which are molecules produced by living organisms. For examples amino acids for the most part only exists in the so called Lenantiomer form and naturally occurring carbohydrates only exist in the so called Denantiomer form (Biochemists use D vs L which is a similar system to the R vs S system that organic chemists use). This shows that it is important for chemists to be able to correctly assign configurations to chirality centers to distinguish these molecules. In the Organic Chemistry I course, a chirality center is generally defined as a carbon that is attached to four distinct groups. These four groups are ranked from highest to lowest priority according to the Cahn-Ingold-Prelog (CIP) convention. According to the CIP convention, the higher priority groups would be ones that are immediately attached to the higher atomic number atom. In the case of ties, the first point of difference in the subsequent set of attached atoms would be considered to assign priority. Once the priorities are assigned to groups, the molecule is oriented such that the lowest priority group is pointing away in space and the direction tracing through the first, second, then third priority groups determine the configuration of the chirality center. A clockwise

direction means R-configuration whereas a counterclockwise direction means Sconfiguration.

Isomers refer to different compounds with the same molecular formula. Stereoisomers are a subclass of isomers that have the same connectivity but have different spatial arrangement of atoms. In the tutorial, three classes of stereoisomers were discussed: enantiomers, diastereomers, and meso compounds. Enantiomers are a pair of stereoisomers that are non-superimposable, mirror images. Diastereomers are a pair of stereoisomers that are non-superimposable, non-mirror images. Meso compounds are achiral molecules that contain chirality centers. One method of determining the relationships between a pair of stereoisomers is to assign R/S on each of the chirality centers and comparing respective chirality centers to see if the configurations are retained or inverted. If the configuration of every chirality center was inverted in a stereoisomer with no symmetry, the resulting stereoisomer would be an enantiomer. If a molecule has chirality centers but also has symmetry, it is a meso compound. If the configuration of some, but not all, chirality centers were inverted in a stereoisomer, the resulting stereoisomer would be a diastereomer.

3.2 R/S Configurations and Stereoisomers Application in VR

From the Organic Chemistry I curriculum, we selected the topic of determining the configurations of chirality centers and determining relationships between stereoisomers as suitable for the development of a VR tutorial. Since stereoisomers are isomers with the same connectivity and different spatial arrangement of atoms in 3D

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space, this topic would best utilize the interactive and immersive experience with the 3D molecules provided in VR.

Similarly to the Diels-Alder Tutorial, features in the R/S Configurations and Stereoisomers tutorial include presentation of topics on a UI, interactive molecules, multiple choice questions to check for understanding, and adaptive release. The tutorial curriculum was developed based on my past three years of experience tutoring organic chemistry and some explanations were taken from Professor Lashley's lecture notes with her permission to minimize confusion with consistent verbiage between class and the tutorial content. The layout of the topics was as follows: relevance of stereochemistry in a biological context, how to identify a chirality center, how to rank priorities of groups attached to the chirality center following the CIP convention, assigning configurations to chirality centers, an introduction to stereoisomers, and an indepth discussion of enantiomers, diastereomers, and meso-compounds.

Multiple choice questions were integrated throughout the presentation of topics, checking if students understood the subtopic necessary for the subsequent exercises. Multiple choice questions were implemented to check if students can identify if a molecule has chirality centers, assign priority rankings to groups on chirality centers, assign configurations of chirality centers, and determine relationships between two molecules.

Adaptive release was also implemented, so that students would only be able to continue in the tutorial after they have viewed the correct answer to each of the multiple-choice questions that check for their understanding.

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3.3 R/S Configurations and Stereoisomers Data

Participants

Participants were volunteers (N = 22, 71.4% female) from 114 students enrolled in Professor Dana Lashley's CHEM 206 - Organic Chemistry I section in Spring 2024. Trials were advertised as an optional help session, which would provide an extra opportunity to engage with determining configurations of chirality centers and stereoisomers before their midterm exam. Various one-hour sessions were available for students to sign up between March $18^{th}-24^{th}$, students were randomly assigned to either the VR learning group (N = 11) or the traditional learning group (N = 10). One data point was omitted because the student did not follow directions and responses were compromised as a result.

Measures

We conducted a pre-survey and a post-survey with a questionnaire developed with Qualtrics. In the pre-survey, we collected demographic data of the students' major, race and ethnicity, gender identity, international student status, and neurodiversity status.

We also measured the comfort level of their understanding of determining configurations of chirality centers and determining relationships between stereoisomers prior to the help session on a scale of 1-7, 1 being extremely uncomfortable and 7 being extremely comfortable.

In the post-survey, we asked what learning group the student was assigned and if they have prior experience in using VR. We measured their enjoyment level during the help session on a scale of 1-7, 1 being extremely unenjoyable and 7 being extremely enjoyable for both topics. We also measured the comfort level of both topics after the help session on a scale of 1-7, 1 being extremely uncomfortable and 7 being extremely comfortable. Students also answered two multiple choice questions on determining relationships between stereoisomers as part of the post-survey. Finally, students were presented with one multiple choice question on determining relationships between stereoisomers timed for three minutes to simulate on-paper exam conditions.

Procedure

The procedure for data collection used for the Diels-Alder tutorial data collection was followed for data collection for the R/S Configurations and Stereoisomers Tutorial.

Data Analytic Plan

Paired samples t-tests were conducted to determine if there was a difference in the comfort levels regarding determining configuration of chirality centers and determining relationships between stereoisomers before and after the tutorial for the combined group of students from both the VR learning and traditional learning groups, the VR learning group, and the traditional learning group.

Independent samples t-tests were conducted to determine if there was a difference in enjoyment levels during two topics of the R/S Configurations and Stereoisomers tutorial as well as a difference in average comfort level score improvement before and after the tutorial between the VR learning group and the traditional learning group.

Factorial ANOVA were conducted to determine if there was a difference in enjoyment levels during learning about both topics for students of different ethnic groups or gender identity groups in VR learning group or traditional learning group. Factorial ANOVA were also conducted to determine if there was a difference in average comfort level score improvement before and after the tutorial for both topics for students of different ethnic groups or gender identity groups in VR learning group or traditional learning group.

3.4 R/S Configurations and Stereoisomers Data Analysis

Subjective Performance in Determining Configuration of Chirality Centers

Paired samples t-tests revealed statistically significant differences in the comfort levels of students in the combined group of students from both the VR learning and traditional learning groups. Student reported comfort levels were higher after the tutorial (M = 5.762, SD = 0.769) than comfort levels before the tutorial (M = 4.619, SD = 1.071), t(20) = -5.754, p < 0.05, two tailed test, d = -1.256. Paired samples t-tests also revealed statistically significant differences in the comfort levels of students in the VR learning group. The comfort levels of students in the VR learning group after the tutorial were higher (M = 5.909, SD = 0.701) than comfort levels before the tutorial (M = 4.727, SD = 1.009), t(10) = -3.634, p < 0.05, two tailed test, d = -1.096. Paired samples t-tests also revealed statistically significant differences in the comfort levels of students in the traditional learning group. The comfort levels of students in the traditional learning group after the tutorial were higher (M = 5.600, SD = 0.843) than comfort levels before the tutorial (M = 4.500, SD = 1.179), t(9) = -4.714, p < 0.05, two tailed test, d = -1.491. We concluded that students in general found the tutorial helpful in their understanding of determining configuration of chirality centers, regardless of tutorial mode. We also concluded that the students in the VR learning group and traditional learning group

thought the respective tutorial modes to have helped in their understanding of

	Mean	Std. Dev.	Mean	Std. Dev.	Calculated t-
	Before	Before	After	After	value
Combined Group	4.619	1.071	5.762	0.769	-5.754*
VR Learning	4.727	1.009	5.909	0.701	-3.634*
Group					
Traditional	4.500	1.179	5.600	0.843	-4.714*
Learning Group					

determining configuration of chirality centers. Data is summarized in Table 3.1.

Table 3.1. Comfort Levels Before and After for Determining Configurations. Statistically significant t-values are noted with *, $\alpha = 0.05$.

Independent samples t-tests revealed statistically significant differences in the reported enjoyment level during this topic of the tutorial between the VR learning group or the traditional learning group. Students in the VR learning group reported higher enjoyment levels during this topic of the tutorial (M = 6.000, SD = 0.632) than students in the traditional learning group (M = 5.000, SD = 1.054), t(19) = -2.666, p < 0.05, twotailed test, d = -1.165. Independent samples t-test revealed no statistically significant differences in the average comfort level score improvement before and after for this topic of the tutorial between the VR learning group (M = 1.182, SD = 1.078) and the traditional learning group (M = 1.100, SD = 0.738), t(19) = -0.201, p > 0.05, two-tailed test. We concluded that in general, students in the VR learning group reported that they enjoyed learning about determining configuration of chirality centers more than the students in the traditional learning group. We were unable to conclude if there were any differences between the different learning groups in how much comfort levels increased before and after learning about determining configuration of chirality centers. Data is summarized in Table 3.2.

	VR Mean	VR Std. Dev.	Traditional	Traditional	Calculated
			Mean	Std. Dev.	t-value
Enjoyment	6.000	0.632	5.000	1.054	-2.666*
Average	1.182	1.078	1.100	0.738	-0.201
Comfort					
Level					
Improvement					

Table 3.2. Enjoyment and Average Comfort Improvement for Determining Configurations. Statistically significant t-values are noted with *, α = 0.05.

Factorial ANOVA revealed no significant difference in the enjoyment levels during this topic of the tutorial for students of different ethnicities experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of ethnicity [F(2, 15) = 0.420, p > 0.05], no significant main effect of learning group [F(1, 15) = 3.439, p >

0.05], and no significant interaction [F(2, 15) = 0.136, p > 0.05]. Data is summarized in

Table 3.3

Learning Group	European White	Non-European	Mixed Ethnicity	Row Means
	vvnite	vvnite		
Traditional	5.000	4.750	5.500	5.083
VR	6.167	5.750	6.000	5.972
Column Means	5.583	5.250	5.750	

Table 3.3. Enjoyment Levels in Determining Configurations by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in the improvement of

comfort levels after this topic of the tutorial for students of different ethnicities

experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of

ethnicity [F(2, 15) = 0.258, p > 0.05], no significant main effect of learning group [F(1, 1)]

15) = 0.069, p > 0.05], and no significant interaction [F(2, 15) = 0.087, p > 0.05]. Data is

summarized in Table 3.4.

Learning Group	European	Non-European	Mixed Ethnicity	Row Means
	White	White		
Traditional	1.250	1.250	0.500	1.000
VR	1.167	1.250	1.000	1.139
Column Means	1.208	1.250	0.750	

Table 3.4. Average Comfort Improvement in Determining Configurations by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in enjoyment levels

during this topic of the tutorial for students of different genders experiencing either

tutorial mode. The 2x3 ANOVA revealed no significant main effect of gender [F(2, 16) =

0.000, p > 0.05], no significant main effect of learning group [F(1, 16) = 4.151, p > 0.05],

and no significant interaction [F(1, 16) = 0.000, p > 0.05]. Data is summarized in **Table**

3.5.

Learning Group	Female	Male	Non-binary	Row Means
Traditional	5.000	5.000	Not Observed	5.000
VR	6.000	6.000	6.000	6.000
Column Means	5.500	5.500	6.000	

Table 3.5. Enjoyment Levels in Determining Configurations by Gender and Learning Group. Statistically significant differences in mean are noted with *, $\alpha = 0.05$.

Factorial ANOVA also revealed no significant difference in the improvement of

comfort levels after this topic of the tutorial for students of different genders

experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of

gender [F(2, 16) = 0.398, p > 0.05], no significant main effect of learning group [F(1, 16)]

= 0.337, p > 0.05], and no significant interaction [F(1, 16) = 1.163, p > 0.05]. Data is

summarized in Table 3.6.

Learning Group	Female	Male	Non-binary	Row Means
Traditional	1.250	0.500	Not Observed	0.875
VR	1.000	1.333	2.000	1.444
Column Means	1.125	0.917	2.000	

Table 3.6. Average Comfort Improvement in Determining Configurations by Gender and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

We concluded that the ethnicity or gender of the student seems to not have an effect on how much the students enjoy VR or traditional learning nor does ethnicity or gender have an effect on how much more comfortable students feel about the content after VR or traditional instruction for this topic of the tutorial.

Subjective Performance in Determining Relationships between Stereoisomers

Paired samples t-tests revealed statistically significant differences in the comfort levels of students in the overall group. Students reported comfort levels were higher after the tutorial (M = 4.905, SD = 0.995) than comfort levels before the tutorial (M =3.476, SD = 1.250), t(20) = -7.071, p < 0.05, two tailed test, d = -1.543. Paired samples t-tests also revealed statistically significant differences in the comfort levels of students in the VR learning group. The comfort levels of students in the VR learning group after the tutorial were higher (M = 4.909, SD = 0.831) than comfort levels before the tutorial (M = 3.273, SD = 0.786), t(10) = -6.708, p < 0.05, two tailed test, d = -2.023. Pairedsamples t-tests also revealed statistically significant differences in the comfort levels of students in the traditional learning group. The comfort levels of students in the traditional learning group after the tutorial were higher (M = 4.900, SD = 1.197) than comfort levels before the tutorial (M = 3.700, SD = 1.636), t(9) = -3.674, p < 0.05, two tailed test, d = -1.162. We concluded that students in general found the tutorial helpful in their understanding of determining relationships between stereoisomers, regardless of tutorial mode. We also concluded that the students in the VR learning group and traditional learning group thought the respective tutorial modes to have helped in their understanding of determining relationships between stereoisomers. Data is summarized in **Table 3.7**.

	Mean	Std. Dev.	Mean	Std. Dev.	Calculated t-
	Before	Before	After	After	value
Combined Group	3.476	1.250	4.905	0.995	-7.071*
VR Learning Group	3.273	0.786	4.909	0.831	-6.708*
Traditional Learning	3.700	1.636	4.900	1.197	-3.674*
Group					

Table 3.7. Comfort Levels Before and After for Stereoisomer Relationships. Statistically significant t-values are noted with *, $\alpha = 0.05$.

Independent samples t-tests revealed no statistically significant differences in the reported enjoyment level during this topic of the tutorial between the VR learning group (M = 5.636, SD = 0.809) and the traditional learning group (M = 5.200, SD = 1.229), t(19) = -0.970, p > 0.05, two-tailed test. Independent samples t-test also revealed no statistically significant differences in the average comfort level score improvement before and after for this topic of the tutorial between the VR learning group (M = 1.636, SD = 0.809) and the traditional learning group (M = 1.200, SD = 1.033), t(19) = -1.083, p > 0.05, two-tailed test. We were unable to conclude if there were any differences between students in different learning groups while learning about determining relationships between stereoisomers. We were also unable to conclude if there were any differences between the different learning groups in how much comfort levels increased before and after learning about determining relationships of stereoisomers. Data is summarized in **Table 3.8**.

	VR Mean	VR Std. Dev.	Traditional	Traditional	Calculated
			Mean	Std. Dev.	t-value
Enjoyment	5.636	0.809	5.200	1.229	-0.970
Average	1.636	0.809	1.200	1.033	-1.083
Comfort					
Level					
Improvement					

Table 3.8. Enjoyment and Average Comfort Improvement for Stereoisomer Relationships. Statistically significant t-values are noted with *, $\alpha = 0.05$.

Factorial ANOVA revealed no significant difference in the enjoyment levels during this topic of the tutorial for students of different ethnicities experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of ethnicity [F(2, 15) = 1.067, p > 0.05], no significant main effect of learning group [F(1, 15) = 0.426, p > 0.05], and no significant interaction [F(2, 15) = 0.079, p > 0.05]. Data is summarized in

Learning Group	European	Non-European	Mixed Ethnicity	Row Means
	White	White		
Traditional	5.250	4.750	6.000	5.333
VR	5.833	5.250	6.000	5.694
Column Means	5.542	5.000	6.000	

Table 3.9.

Table 3.9. Enjoyment Levels in Stereoisomer Relationships by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in the improvement of

comfort levels after this topic of the tutorial for students of different ethnicities

experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of

ethnicity [F(2, 15) = 0.707, p > 0.05], no significant main effect of learning group [F(1, 1)]

15) = 0.557, p > 0.05], and no significant interaction [F(2, 15) = 0.850, p > 0.05]. Data is

summarized in	1 able 3.10.	

	Ethnicity			
Learning Group	European	Non-European	Mixed Ethnicity	Row Means
	White	White		
Traditional	0.750	1.250	2.000	1.333
VR	1.833	1.250	2.000	1.694
Column Means	1.292	1.250	2.000	

Table 3.10. Average Comfort Improvement in Stereoisomer Relationships by Ethnicity and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in enjoyment levels

during this topic of the tutorial for students of different genders experiencing either

tutorial mode. The 2x3 ANOVA revealed no significant main effect of gender [F(2, 16) =

0.801, p > 0.05], no significant main effect of learning group [F(1, 16) = 0.467, p > 0.05],

and no significant interaction [F(1, 16) = 0.467, p > 0.05]. Data is summarized in **Table**

3.11.

	Gender Identity			
Learning Group	Female	Male	Non-binary	Row Means
Traditional	5.250	5.000	Not Observed	5.125
VR	6.000	5.000	5.000	5.333
Column Means	5.625	5.000	5.000	

Table 3.11. Enjoyment Levels in Stereoisomer Relationships by Gender and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

Factorial ANOVA also revealed no significant difference in the improvement of

comfort levels after this topic of the tutorial for students of different genders

experiencing either tutorial mode. The 2x3 ANOVA revealed no significant main effect of

gender [F(2, 16) = 0.278, p > 0.05], no significant main effect of learning group [F(1, 16)]

= 1.192, p > 0.05], and no significant interaction [F(1, 16) = 0.038, p > 0.05]. Data is

summarized in Table 3.12.

	Gender Identity			
Learning Group	Female	Male	Non-binary	Row Means
Traditional	1.250	1.000	Not Observed	1.125
VR	1.714	1.667	1.000	1.460
Column Means	1.482	1.333	1.000	

Table 3.12. Average Comfort Improvement in Stereoisomer Relationships by Gender and Learning Group. Statistically significant differences in mean are noted with *, α = 0.05.

We concluded that the ethnicity or gender of the student seems to not have an

effect on how much the students enjoy VR or traditional learning nor does ethnicity or

gender have an effect on how much more comfortable students feel about the content

after VR or traditional instruction for this topic of the tutorial.

Content Performance

Like from the Diels-Alder data collection, we kept records of content performance with the check for understanding questions and the on-paper exam simulation. Check for understanding question 1 (**Figure 3.1**) had an overall correct response rate of 0.333 (7/21), the VR learning group had a correct response rate of 0.364 (4/11), and the traditional learning group had a correct response rate of 0.300 (3/10).

Q1. Determine the relationship between the following pair of molecules (circle one)





Figure 3.1. Multiple-Choice Check for Understanding Question 1 for R/S Configurations and Stereochemistry. Enantiomers is the correct answer.

Check for understanding question 2 (**Figure 3.2**) had an overall correct response rate of 0.571 (12/21), the VR learning group had a correct response rate of 0.636 (7/11), and the traditional learning group had a correct response rate of 0.500 (5/10). Q2. Determine the relationship between the following pair of molecules (circle one)





Figure 3.2. Multiple-Choice Check for Understanding Question 2 for R/S Configurations and Stereochemistry. Diastereomers is the correct answer.

The on-paper exam simulation (**Figure 3.3**) had an overall correct response rate of 0.190 (4/21), the VR learning group had a correct response rate of 0.182 (2/11), and the traditional learning group had a correct response rate of 0.200 (2/10). We were unable to conclude if there were any differences in learning outcome between the students of different learning groups.





Figure 3.3. Multiple-Choice Check for On-Paper Exam Simulation for R/S Configurations and Stereochemistry. Identical molecules is the correct answer.

Data on content performance for R/S Configurations and Stereoisomers is summarized in Table **3.13**.

	Overall	VR	Traditional
Question 1	0.333	0.364	0.300
Question 2	0.571	0.636	0.500
Exam Simulation	0.190	0.182	0.200

Table 3.13. Correct Response Rates for Content Performance in R/S Configurations and Stereoisomers.

3.5 Possible Sources of Error for R/S Configurations and Stereoisomers Tutorial

Although data collection was conducted at a more optimal timeframe, before students were formally tested on determining configuration of chirality centers and determining relationships of molecules, we suspect that the check for understanding guestions were too difficult to accurately assess if students understood the presented material. It is possible that student performances on the check for understanding guestions did not have a statistically significant difference between the VR learning group and traditional learning group because the problems were too difficult even for students who had a good understanding of the content. Based on the correct response rates of 0.33, 0.57, and 0.19 on the three questions with four choices available, we can reasonably infer that the questions were too difficult. It is also possible that our data is underestimating how comfortable students felt about the topics in the tutorials because the post-survey was designed on one page, so the questions asking about comfort levels on the topic after the tutorial were presented on the same page as the challenging check for understanding questions. If some students felt discouraged after answering the questions, they could have changed their responses to the comfort level questions, which could have resulted in a decreased average score than what we expected after the tutorials.

Chapter 4 Conclusion and Future Outlook

4.1 Conclusion

Although we were unable to conclude if VR learning in organic chemistry leads to improved student performances on exam-like questions compared to traditional learning, we saw that students in the VR learning group generally reported higher enjoyment during the help session than students in the traditional learning group. From the survey free response feedback, many students also showed excitement for the VR tutorial and found the tutorials to be a "cool and enjoyable" experience. This indicates that while VR learning cannot completely replace traditional learning in organic chemistry education, it shows potential as a supplemental learning tool by increasing student interest and engagement. We observed these trends in both the Diels-Alder tutorial and the R/S Configurations and Stereoisomers tutorial, which we thought was promising that VR can be helpful as a teaching supplement for both organic chemistry I and II topics. Our data also seems to suggest that the ethnicity or gender of the students does not affect the efficacy of the VR tutorials, so VR may also be useful as an equitable learning supplement. Considering that we had no prior knowledge in VR development before this project but still obtained deliverable projects that resulted in similar learning outcomes to traditional learning seems promising to future developers who might be interested in developing supplemental VR tutorials to fit their class material.

4.2 Future Outlook on VR

Improvements for Developed Products

Due to limited time in development, there were some features in each tutorial that we were unable to implement that could have further enhanced the learning experience of the students.

In the Diels-Alder tutorial, we wanted to implement an undo reaction button, so that students could redo the reactions multiple times to understand how the starting materials combine to yield the reaction products. We also wanted to discuss the regiochemistry of Diels-Alder reaction in addition to the stereochemistry to present a more comprehensive tutorial. We also wanted to show the newly formed pi bond of the products so that students could more easily visualize how part of the diene and the dienophile came together to make the product. From the survey feedback, students also requested to show more example questions and to cover more depth for topics like electron orbital theory, requirements for the diene, and discussing electron withdrawing and donating groups for regiochemistry. Students also suggested quality of life improvements such as highlighting new bonds, making double bonds clearer, and coloring the "outside" and "inside" substituents on the diene with different colors.

In the R/S Configurations and Stereoisomers tutorial, we wanted to highlight the chirality center of the molecule in a different color to reduce confusion when students are looking at the molecule. We also wanted to highlight specific atoms in a molecule for discussing priority rankings to assign configuration of the chirality center. The ability to highlight a given atom could have provided clearer information to the students. This was unable to be implemented in time because Atomic Blender Utilities does not seem to

allow selection of just one atom if there are multiple atoms of the same element, so changing the color of one atom would change the color of every atom of the same element. From the student feedback, we could make quality of life improvements to make the flow charts and graphics less blurry, reminders to also look at the 2D drawings after looking at the 3D models to facilitate the transition back to classroom learning, and indicators for how many slides are left in the tutorial.

Possible Unexplored Topics for VR

Although we only have finished products for reinforcing reaction mechanisms and 3D visualization heavy topics, we also had instrument/lab equipment tutorials in mind as possible topics for developing VR. Instruments and lab equipment used in organic chemistry labs, such as the Gas Spectrometer or the rotational evaporator ("rotovap"), can be daunting for first time users. Making a mistake when using an instrument while working with toxic chemicals can be costly, and the instrument itself can also be costly to repair or replace if damaged from the mistakes. We think that VR tutorials for such lab equipment/instrument could help overcome the fear of using unfamiliar instruments and equipment for first time organic chemistry lab students. Lab techniques that require extensive set up such as distillation and reflux might also be appealing topics for a VR tutorial. An easier method of developing a lab equipment/instrument tutorial could be the VR developer carrying out the lab themselves, demonstrating how to properly handle the equipment while filming a 360-degree video with a GoPro or similar equipment attached to their forehead. The resulting footage can be incorporated into the VR environment for the students to view the motions from a first-person perspective. For such lab tutorials, the ultimate goal could be to have interactive lab apparatus simulation

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for every complex piece of equipment for the lab that students interact with. The students would be able to manipulate and interact with the equipment in VR in any way imaginable and the VR would have pre-programmed responses to give feedback to all the creative choices a student could make in operating the virtual equipment, maximizing the benefits of creative learning with VR.

4.3 Improvements on Methodology

There are a few improvements to the Diels-Alder and R/S Configurations and Stereoisomers trials if there was more time for this project. More data points for analysis would help in making a stronger conclusion, so recruiting more students or even running the trials for another group of students could improve results. To account for the varying difficulties of the questions in assessing content performance, giving students content questions before the tutorial to compare with their performance after the tutorial could have helped in assessing if students in different learning groups improved their understanding of the content. As an additional measure of efficiency of the different types of tutorials, the time for completing the tutorials could also have been measured. It would also be interesting to investigate if showing 2D drawings along with 3D models in the VR tutorial affects learning outcomes for either the Diels-Alder tutorial or the R/S Configurations and Stereoisomers tutorial.

Appendix

Section A – StudentIRB Approval

This research collected data from students, so it is categorized as a human subjects research, and requires approval from the Protection of Human Subjects Committee (PHSC) or StudentIRB. Since this research was conducted in a commonly accepted educational setting of optional help session and involved normal educational practices that likely did not adversely impact students' opportunity to learn, the research was eligible for exempt research¹⁰. Exempt research poses no more than minimal risk to the participants, and the protocol for the research should be sent to StudentIRB for review rather than to the PHSC¹¹. Items to submit with the protocol include: the informed consent form for the participants detailing the purpose of the study, procedure, possible risks and benefits, statement of confidentiality, statement of voluntary participation, incentive for participation, and contact information of the investigators, the list of survey questions for the participants, and relevant CITI training certificates for every investigator.

Section B - Software and Hardware used for VR Development

The Meta Quest 2 headset was chosen as the VR headset and tutorials were developed with the Unity game engine (version 2022.3.2f1). The VR environment and functions were part of the Create-with-VR file under the Create with VR course available on Unity Learn, adapted to suit the tutorials. 3D models of molecules were built with Avogadro2 and Blender (Version 4.0). Unity Hub, Meta Quest Developer Hub, and the Oculus PC app were installed, and a Quest Link Cable as well as a Meta Quest Link Cable developer account was acquired. Unity Hub, Oculus PC app, and the Quest Link Cable

were used for developing and testing the VR with Unity, and the Meta Quest Developer Hub and the Meta Quest developer account were used for distributing the finished tutorials.

Section C – Importing 3D Molecules

To import the desired 3D molecules, we used Avogadro2, a software for editing and visualizing chemicals¹². When building the molecules, we either drew the molecule from scratch in Avogadro2, or we imported the molecule using the Simplified Molecular Input Line Entry System (SMILES). Drawing the molecule from scratch works well with smaller molecules, while using SMILES works well with larger molecules. One caveat for importing molecules with SMILES is that have to check if the molecule imported with the desired stereochemistry, as there does not seem to be a reliable way of importing different stereoisomers or choosing the correct stereoisomer with SMILES, which often led to editing the molecule after importing them. After importing the molecules, we standardized the appearance of the molecules by **Extensions -> Open Babel->**

Optimize Geometry. After adjusting the molecule in Avogadro2, we exported the molecule as a Protein Data Bank (.pdb) file by File -> Export -> Molecule and saving as filename.pdb. Then we imported the saved file into Blender, a 3D computer graphics software by selecting File -> Import -> Protein Data Bank (.pdb). We want to be sure to select the Bonds checkbox under the Sticks/bonds menu to show any double or triple bonds in the molecule. Select the desired molecule file and click Import Protein Data Bank. To edit the molecules in Blender, we need an add-on, which we can obtain from Edit-> Preferences and selecting Import-Export: Atomic Blender PDB/XYZ under the Add-ons tab. Under the Import-Export: Atomic Blender PDB/XYZ dropdown menu,

select PDB import/export and Utility panel. This creates a panel called Atomic Blender Utilities under the Create tab on the right side of the Blender interface where we can customize the atomic radii and bond sizes. Before exporting the molecule, we can also orient the molecule according to the xyz coordinate directions, which will become the local xyz coordinates for the molecule in Unity. To export the molecule, **File** -> Export -> FBX (.fbx) and select Visible Objects under the Include dropdown. Select Export FBX to save the molecule. Now these .fbx molecule files are available to be uploaded into the Unity game engine as GameObjects.

Section D - Making 3D Molecules Interactable Objects

Drag the 3D molecule fbx file into the **Hierarchy** region of Unity, this makes the 3D molecule a GameObject that can be manipulated in Unity. The size of the 3D molecule can be adjusted from the **Inspector** of the GameObject by assigning different values in the **Scale** under **Transform** component. To the 3D molecule GameObject, add the **Rigidbody** component, a **Collider** component (such as a **Box Collider**), and the **XR Grab Interactable** component. In the **Rigidbody** component, change the **Collision Detection** to **Continuous Dynamic**. For the **XR Grab Interactable** component, change the **Movement Type** to **Kinematic** and nothing else has to be modified if the orientation of the molecule does not matter when it is grabbed. If there is a desired orientation when the molecule is grabbed, add an empty GameObject to the 3D molecule GameObject under the **Hierarchy** region by right clicking -> **Create Empty** and orient the empty GameObject appropriately. Under the **XR Grab Interactable** component, drag and drop the new empty GameObject into **Attach Transform**. For the **Collider** component, select the type of Collider that would best encompass the outline of the molecule, and edit the outline with the **Edit Collider** button and adjust the outlines.

Section E - Making Reactions Between Molecules

To make reactions happen when molecules are in contact or in close proximity, a hitbox is required. Under the **Hierarchy** region of Unity, create an empty GameObject to the 3D molecule by right clicking -> **Create Empty.** In the **Inspector** of the empty GameObject, add a type of **Collider** component and check the **Is Trigger** box. Adjust the collider size with the **Edit Collider** button and adjust the outlines. Also add the **On Trigger (Script)** component and under **On Enter (Collider)**, add all the actions that should happen when the molecules make contact (e.g. the reactant molecules are set as inactive, the product molecules are set as active, and the Continue button is set as active).

Section F - Making and Linking UI Panels

For the main panel, right click the **Hierarchy** region, **XR** -> **UI Canvas**. Drag the **Main Camera (Camera)** under **Event Camera** in the **Inspector** of the **UI Canvas**. Set the **Order in Layer** as 1. This main panel will serve like a projector screen for the other panels. For the panels, right click the **Hierarchy** region, **UI** -> **Panel**. These are like individual slides on which we can put text, buttons, and images to design our VR tutorial. For text, right click the panel, **UI** -> **Text - TextMeshPro** and type the content in the **Inspector** region under **Text Input**. For an image, right click the panel, **UI** -> **Image** and drag and drop the desired image to the **Source Image** under the **Image** component in the **Inspector region**. Note that the image should be modified by going to the **Inspector** of the image, going to **Texture Type** and selecting **Sprite (2D and UI)**. To

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make a button, right click the panel, **UI** -> **Button - TextMeshPro**. The button has a built in Text object that can be modified, and actions for when the button is clicked can be set in the **Inspector** region, by adding actions to **On Click ()**, where actions such as setting the current panel as inactive, setting the next panel as active, and making certain buttons active can be set up to employ adaptive release.

Section G - Uploading to the Headset

To upload and test on a Meta Quest 2 headset that has enabled developer mode, the VR headset can be tethered to the computer with the Quest Link Cable and Oculus PC app. Disabling the XR Device Simulator and clicking **Play** in Unity projects the VR environment to the headset for quick testing and modifying of the simulation in development. To test the product without being tethered to the computer, the simulation must be built into the headset. While the VR headset is connected to the computer, go to **File** -> **Build Settings**. Select **Android** under **Platform** and select the VR headset under **Run Device**. Click **Build** and save the product as a .apk file on the computer. When the build is finished, the product should be available in the VR headset when navigating to Apps and under **Unknown Sources** from the dropdown menu.

Section H - Making the App Available for Other Headsets

To make the product available for other headsets that does not have developer mode, the product has to be made into an application. Publishing an application on the official VR app store is very lengthy and rigorous, another method had to be used to fit the timescale of this project. Meta Quest has a secondary app store called App Lab for distributing apps in development by a distribution link. First, log into the Oculus Developer Dashboard with the developer account, click **Create New App** and select Meta Quest (App Lab). To build the .apk file, go to File -> Build Settings and go to Player Settings. Go to the Publishing Settings dropdown menu and set up a Keystore with the **Keystore Manager**. The Keystore serves like a password for making any changes to the app. Under the Other Settings dropdown menu, go to Install Location and select Automatic. Also note that every time the product is built as an .apk file for upload, the Bundle Version Code should be different. Increasing the Bundle Version **Code** by 1 each time a file is built seems to work. Build the .apk file. Navigate to the Meta Quest Developer Hub and click **App Distribution** and the app name. Under the alpha channel, upload the .apk file. Once the build is uploaded, the distribution link can be found on the Oculus Developer Dashboard, go to Distribution -> Release **Channels** and click on the alpha channel then go to **Channel Settings**. There should be a **Channel Invite** and an option to **Grant access to users by URL.** When the users click on the distribution link, they should log into their Meta accounts and accept the invite, then they should be able to download the product to their Meta Quest 2 headsets by searching the exact app name on the Quest store.



Section I - UI Panels for the Diels-Alder Tutorial

Figure I.1. Aerial View of the Diels-Alder Tutorial.



Figure I.2. Welcome Slide and Overview for Diels-Alder Tutorial



Figure I.3. Simplest Case Diels-Alder with no Substituents on the Diene or the Dienophile



Figure I.4. Overview of the Reaction Mechanism with the Simplest Case Diels-Alder Reaction



Figure I.5. First Requirement for the Diene to be s-cis for Diels-Alder



Figure I.6. Second Requirement for the Diene to be Conjugated



Figure I.7. Introduction to Substituents on the Diene and/or the Dienophile



Figure I.8. Example of a Reaction of Substituted Diene and Substituted Dienophile



Figure I.9. Introduction to Bicyclic Products Resulting from a Cyclic Diene



Figure I.10. 2D and 3D Views of the Bicyclic Product from Figure I.9.



Figure I.11. Bicyclic Products Resulting from a Cyclic Dienophile



Figure I.12. 2D and 3D Views of the Bicyclic Product from Figure I.11.


Figure I.13. Stereochemistry Resulting from the Dienophile being cis- or trans-.



Figure I.14. Cis- Substituents on Dienophiles Result Syn- on the Product. This panel shows when "Substituents on the dienophile are cis" is selected from **Figure I.13.**



Figure I.15. Trans- Substituents on Dienophiles Result Anti- on the Product. This panel shows when "Substituents on the dienophile are trans" is selected from **Figure I.13.**



Figure I.16. Example for Stereochemistry Resulting from the Dienophile being cis- or trans-.



Figure I.17. Example for Stereochemistry Resulting from the Dienophile being cis-. This panel shows when "Add the cis-dicarboxylic acid to the diene" is selected from **Figure I.16.**



Figure I.18. Example for Stereochemistry Resulting from the Dienophile being trans-. This panel shows when "Add the trans-dicarboxylic acid to the diene" is selected from **Figure I.16.**



Figure I.19. Stereochemistry from the Diene Substituents being "outside" or "inside".



Figure I.20. Example for Stereochemistry from Diene Substituents being "outside" or "inside".



Figure I.21. Example for Stereochemistry from Diene Substituents being "outside". This panel shows when "Both methyls "outside"" is selected from **Figure I.20.**



Figure I.22. Example for Stereochemistry from Diene Substituents being "outside" and "inside". This panel shows when "One methyl "outside" one methyl "inside"" is selected from **Figure I.20.**



Figure I.23. Intro to Stereochemistry from Both the Diene and Dienophile being Substituted.



Figure I.24. Introduction to Endo- and Exo- Products.



Figure I.25. Description and Example of an Endo- Product.



Figure I.26. Description and Example of an Exo- Product.



Figure I.27. Introduction to Bicyclic Endo- and Exo- Products.



Figure I.28. Examples of Bicyclic Endo- and Exo- Products.



Figure I.29. Example of a Bicyclic Endo- Product.



Figure I.30. Example of a Bicyclic Exo- Product.



Figure I.31. Final Slide of Diels-Alder Tutorial.

Section J - UI Panels for the R/S Configurations and Stereochemistry Tutorial



Figure J.1. Front UI Panel of the R/S Configurations and Stereochemistry Tutorial.



Figure J.2. Supplemental Periodic Table.



Figure J.3. Supplemental Atom Color Chart.

Welcome to the Stereochemistry Tutorial In this exercise, we will explore determining R/S for chirality centers and identifying relationships between stereoisomers. Throughout the tutorial, make sure to interact with the 3D models of molecules to enhance your understanding Before we begin, make sure to locate the periodic table on your right. Continue Interact with the molecules!	

Figure J.4. Aerial View of the R/S Configurations and Stereochemistry Tutorial.



Figure J.5. Introduction to the Relevance of Chirality Centers.



Figure J.6. Introduction to the Relevance of Chirality Centers Continued.



Figure J.7. Introduction to Chirality Centers in Organic Chemistry I.



Figure J.8. Identifying Chirality Centers when Groups have Different Chemical Compositions.



Figure J.9. Identifying Chirality Centers when Groups have Different Branching.



Figure J.10. Example of Groups with Different Branching. This panel shows when "See Example" is selected from **Figure J.9.**



Figure J.11. Identify Chirality Centers when Groups have Different Branching with Continue. The "Continue" button appears after students have viewed **Figure J.10.**



Figure J.12. Example of an Achiral Center.



Figure J.13. Identifying Chirality Centers Practice 1.



Figure J.14. Identifying Chirality Centers Practice 1 Feedback for Yes. This is the incorrect answer. This panel shows when "Yes" is selected from **Figure J.13.**



Figure J.15. Identifying Chirality Centers Practice 1 Feedback for No. This is the correct answer. This panel shows when "No" is selected from **Figure J.13.**



Figure J.16. Identifying Chirality Centers Practice 2.



Figure J.17. Identifying Chirality Centers Practice 2 Feedback for Yes. This is the correct answer. This panel shows when "Yes" is selected from **Figure J.16.**



Figure J.18. Identifying Chirality Centers Practice 2 Feedback for No. This is the incorrect answer. This panel shows when "No" is selected from **Figure J.16.**



Figure J.19. Introduction to R/S Assignment.



Figure J.20. Introduction to Ranking Priority to Groups.



Figure J.21. Priority Ranking Based on Atomic Numbers.



Figure J.22. Priority Ranking Based on Isotopes.



Figure J.23. Priority Ranking with Point of First Difference.



Figure J.24. Priority Ranking with Point of First Difference Example.



Figure J.25. Priority Ranking with Point of First Difference Example Continued.



Figure J.26. Priority Ranking with Double and Triple Bonds.



Figure J.27. Priority Ranking with Double and Triple Bonds Continued.



Figure J.28. Priority Ranking Practice Multiple-Choice Question 1.



Figure J.29. Priority Ranking Practice Multiple-Choice Question 1 Choice A. This is an incorrect answer. This panel shows when "A) IV, III, II, I" is selected from **Figure J.28.**



Figure J.30. Priority Ranking Practice Multiple-Choice Question 1 Choice B. This is the correct answer. This panel shows when "B) IV, III, I, II" is selected from **Figure J.28**.



Figure J.31. Priority Ranking Practice Multiple-Choice Question 1 Choice C. This is an incorrect answer. This panel shows when "C) I, IV, III, II" is selected from **Figure J.28.**



Figure J.32. Priority Ranking Practice Multiple-Choice Question 2.



Figure J.33. Priority Ranking Practice Multiple-Choice Question 2 Choice A. This is an incorrect answer. This panel shows when "A) III, I, II, IV" is selected from **Figure J.32.**



Figure J.34. Priority Ranking Practice Multiple-Choice Question 2 Choice B. This is an incorrect answer. This panel shows when "B) II, I, III, IV" is selected from **Figure J.32**.



Figure J.35. Priority Ranking Practice Multiple-Choice Question 2 Choice C. This is the correct answer. This panel shows when "C) II, III, I, IV" is selected from **Figure J.32.**



Figure J.36. How to Properly Orient Molecules.



Figure J.37. Assigning R or S.



Figure J.38. Practice R/S Question 1.



Figure J.39. Practice R/S Question 1 Choice R. This is the correct answer. This panel shows when "R" is selected from **Figure J.38.**



Figure J.40. Practice R/S Question 1 Choice S. This is the incorrect answer. This panel shows when "S" is selected from **Figure J.38.**



Figure J.41. Practice R/S Question 2.



Figure J.42. Practice R/S Question 2 Choice R. This is the incorrect answer. This panel shows when "R" is selected from **Figure J.41.**



Figure J.43. Practice R/S Question 2 Choice S. This is the correct answer. This panel shows when "S" is selected from **Figure J.41.**



Figure J.44. Introduction to Stereoisomers.



Figure J.45. Overview of Stereoisomers in this Tutorial.



Figure J.46. Determining the Maximum Number of Stereoisomers.



Figure J.47. Determining the Maximum Number of Stereoisomers Example.



Figure J.48. Introduction to Enantiomers.



Figure J.49. Introduction of Enantiomers as Chiral Molecules.



Figure J.50. Example of Enantiomers 1 with Question.



Figure J.51. Example of Enantiomers 1 Question Choice Left. This is the correct answer. This panel shows when "Left Stereoisomer" is selected from **Figure J.50.**



Figure J.52. Example of Enantiomers 1 Question Choice Right. This is the incorrect answer. This panel shows when "Right Stereoisomer" is selected from **Figure J.50.**


Figure J.53. Example of Enantiomers 2.



Figure J.54. Introduction to Diastereomers.



Figure J.55. Example of Diastereomers 1.



Figure J.56. Example of Diastereomers 2.



Figure J.57. Relationship between the Four Stereoisomers.



Figure J.58. Introduction to Meso Compounds.



Figure J.59. Enantiomer Pair of Stereoisomers. One molecule is R,R and the other molecule is S,S.



Figure J.60. Meso Compound Pair of Stereoisomers.



Figure J.61. Relationship between Meso Compound and Enantiomer Pair.



Figure J.62. Relationship between Meso Compound and Enantiomer Pair Continued.



Figure J.63. How to Identify Meso Compounds.



Figure J.64. Introduction to Plane of Symmetry.



Figure J.65. Relationship Between Stereoisomers Question 1.



Figure J.66. Relationship Between Stereoisomers Question 1 Choice Enantiomer. This is an incorrect choice. This panel shows when "Enantiomers" is selected from **Figure J.65.**



Figure J.67. Relationship Between Stereoisomers Question 1 Choice Diastereomer. This is the correct choice. This panel shows when "Diastereomers" is selected from **Figure J.65.**



Figure J.68. Relationship Between Stereoisomers Question 1 Choice Meso Compound. This is an incorrect choice. This panel shows when "Meso Compounds" is selected from **Figure J.65.**



Figure J.69. Relationship Between Stereoisomers Question 2.



Figure J.70. Relationship Between Stereoisomers Question 2 Choice Enantiomer. This is an incorrect choice. This panel shows when "Enantiomers" is selected from **Figure J.69.**



Figure J.71. Relationship Between Stereoisomers Question 2 Choice Diastereomer. This is an incorrect choice. This panel shows when "Diastereomers" is selected from **Figure J.69.**



Figure J.72. Relationship Between Stereoisomers Question 2 Choice Meso Compound. This is the correct choice. This panel shows when "Meso Compounds" is selected from **Figure J.69.**



Figure J.73. Relationship Between Stereoisomers Question 3.



Figure J.74. Relationship Between Stereoisomers Question 3 Choice Enantiomer. This is the correct choice. This panel shows when "Enantiomers" is selected from **Figure J.73.**



Figure J.75. Relationship Between Stereoisomers Question 3 Choice Diastereomer. This is an incorrect choice. This panel shows when "Diastereomers" is selected from **Figure J.73.**



Figure J.76. Relationship Between Stereoisomers Question 3 Choice Meso Compound. This is an incorrect choice. This panel shows when "Meso Compounds" is selected from **Figure J.73.**



Figure J.77. Final Slide of R/S Configurations and Stereoisomers Tutorial

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