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Journal:	*Journal of Chemical Education*
Manuscript ID	ed-2018-00145d.R1
Manuscript Type:	Activity
Date Submitted by the Author:	n/a
Complete List of Authors:	Winfield, Leyte; Spelman College, Chemistry McCormack, Kai; Spelman College, Chemistry Shaw, Tiana; Spelman College, Chemistry
Keywords:	Second-Year Undergraduate < Audience, Organic Chemistry < Domain, Hands-On Learning / Manipulatives < Pedagogy, Inquiry-Based / Discovery Learning < Pedagogy, Alkanes / Cycloalkanes < Topics, Conformational Analysis < Topics, Molecular Modeling < Topics, Molecular Properties / Structure < Topics, Computer-Based Learning < Pedagogy

PUBLICATION TYPE: Activity

Using iSpartan to support a student-centered activity on alkane conformations

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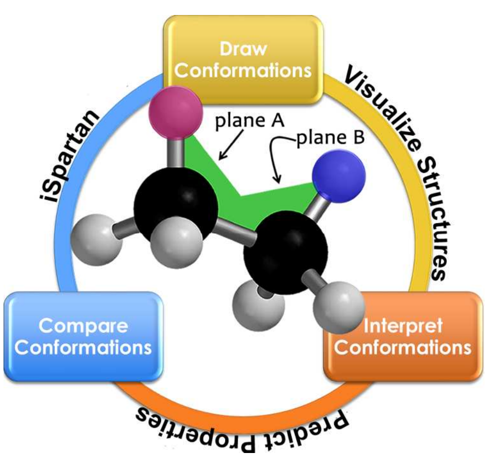
ABSTRACT

Strategies employed in the organic chemistry course must have the shared benefit of promoting concept mastery and visual literacy. With this in mind, an iSpartan-enabled visualization and computational activity was developed to complement learning in the first-semester organic chemistry course. The activity provides students an opportunity to draw molecules, collect structure-based data, and engage in group discussions related to acyclic alkane conformations. Students do not receive a lecture or complete required reading on conformations. Instead, the activity along with group and instructor facilitated discussions serves as the method of content delivery for the topic. Pre- and post-test scores suggest improvements in students' ability to interpret Newman Projections and determine relative conformation energies and stabilities. A survey was administered to determine the degree to which students valued the activity and the associated technology, the response to which suggests that the activity was instrumental in students' ability to comprehend and apply concepts related to alkane conformation.

GRAPHICAL ABSTRACT



KEYWORDS
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Research demonstrates that student-centered instruction, when employed thoughtfully and systematically, provides more favorable learning gains in comparison to traditional lecture techniques.[1-4] Such instruction can encompass a wide variety of pedagogies including inquiry-, problem-, case-, and team-based approaches. Each promotes meaningful course engagement, with students being actively involved and controlling their learning process.[5] The activity described here capitalizes on the hallmarks of student-centered instruction by allowing students to advance their understanding of alkane conformations by investigating relevant trends that are traditionally obtained through a lecture or course reading.

In organic chemistry, student-centered instruction is enhanced by the use of dynamic models that help students create accurate mental images of molecular phenomena and derive meaning from structural data.[6-14] Learning concepts related to alkane conformations, in particular, can be complicated by the simultaneous need to demonstrate visual literacy and representational competency.[11-12, 15-16] Viewing three-dimensional models may reduce the cognitive load imposed on students' memories when approaching problems that require an understanding of such structural information.[11, 17-18] Therefore, tools that allow for the visualization and manipulation of structures, such as iSpartan, can aid a student's mastery of concepts like alkane conformations.

Uses for iPads in the chemistry curriculum continue to expand to support paperless classrooms, collaborative learning, and visual and computational activities.[18-24] The touch-screen technology coupled with platforms for viewing three-dimensional structures is a beneficial tool for teaching visual concepts.[25] The use of iSpartan[26-27] has emerged in the literature within the past five years, although the full and textbook versions of Spartan have been widely used for pedagogical purposes.[28-33] The activity described herein gives students the opportunity to manipulate dynamic models in a three-dimensional space using the iSpartan app.

THE ACTIVITY

The activity was implemented in the Fall 2013 – Fall 2016 first-semester, organic chemistry lecture. The activity uses the iSpartan app (Wavefunction, Inc.; Irvine, CA), which runs on the iPad (Apple, Inc.; Cupertino, CA). A classroom set of iPads (40 total) was used, allowing each student in a group to have an iPad. The instructor created structures using Spartan (version 10; Wavefunction, Inc.; Irvine, CA). The structures were distributed to students through a shared drive (Dropbox, Inc.; San Francisco, CA).

The iSpartan activity was completed in four parts, over the course of three class periods (Table 1). Instructions and follow-up questions for each part were organized into four worksheets (Supporting Information). Students received a summary of expected learning objectives (Table 1). Specific concepts related to alkane conformations were introduced through the completion of the activity and related discussions. Students initially attempted each worksheet alone before discussing the solutions in groups of 4 – 5 students. The instructor was available to explain how to interpret the iPad structures and calculate properties. The instructor also monitored group discussion and answered questions when needed. A class discussion was facilitated by the instructor to confirm solutions and ensure comprehension of the information presented in each worksheet. During the discussion, group members presented their answers and provided an explanation that was affirmed or corrected by the instructor.

Table 1. Components of the activity and related learning objectives.

Part	Worksheet	Learning Objectives
1	Translating representations	Be able to draw three-dimensional structural representations (Newman, wedge-dash, or sawhorse projections) based on: – the IUPAC name – a two-dimensional representation (bond-line or condensed formula) – a different three-dimensional representation
2	Ethane	Be able to: – define gauche, anti, and eclipsed conformations – explain the stability of the conformation based on the orientation of the selected hydrogen atoms and the energy of the conformation
3	Ethane versus butane	Be able to explain and compare the stability of a conformation

		based on substituent size and interactions
4	Butane versus 2,2,5,5-tetramethylhexane	Be able to explain and compare the stability of a conformation based on substituent size and interactions

Before the activity, students completed an online reading assignment and quiz that addressed interpreting energy diagrams (see Supporting Information). In Part 1, students learned to import structures into iSpartan and manipulate the three-dimensional representations generated in the app. The instructor demonstrated how to align the iSpartan structure to thee-dimensional representations (saw-horse, wedge-dash, and Newman projections). Although students had the option of drawing the molecule in iSpartan, students were observed using gestures[25, 34] and mnemonic techniques (see supplemental information) to translate between three-dimensional representations. In addition, students had access to handheld models which some used to confirm what was observed on the iPad screen.

For part 2, students used iSpartan to measure the dihedral angle between the hydrogen atoms designating the eclipse, gauche, and anti substituents of ethane (Figure 1). Students combined the measurements with the information from the reading assignment to discuss the relationship between structural features and calculated properties. Students noted that the terms corresponded to the relative location of the hydrogens on the axis of rotation.

Part 3 allowed students to consider the differences between the conformations of ethane and butane. The angles between designated substituents and the energy of each conformation were provided in the worksheet. Students were able to visualize the relative size of the methane substituent versus the hydrogen substituent using the models included on the worksheet. Therefore, this portion of the activity did not require the use of iSpartan and could be completed outside of class. It is noted that manipulating the three-dimensional representation of butane and calculating the properties in the app would be helpful, but did not occur in this case due to the amount of time allotted for the discussion of this topic. Students were, however, able to manipulate the butane molecule within the app while completing the subsequent worksheet. Students discussed their worksheet responses during the following in-class discussion. Substituent size and interactions were reemphasized in Part 4. The space-filling model was used to illustrate substituent size and steric interactions (Figure 2).

With the instructor facilitating the discussion, students were able to move efficiently through part 4 in one class period.

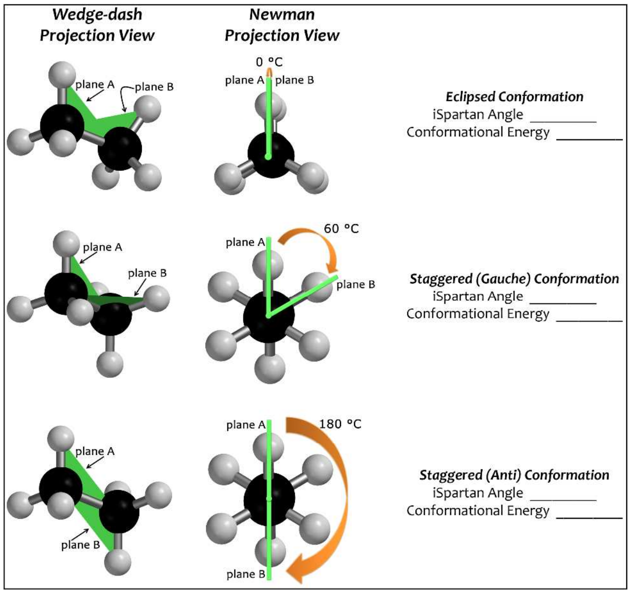

Figure 1. Template for calculating angles and energies in Part 2. The images are aligned to coincide with the wedge-dash and Newman projections.

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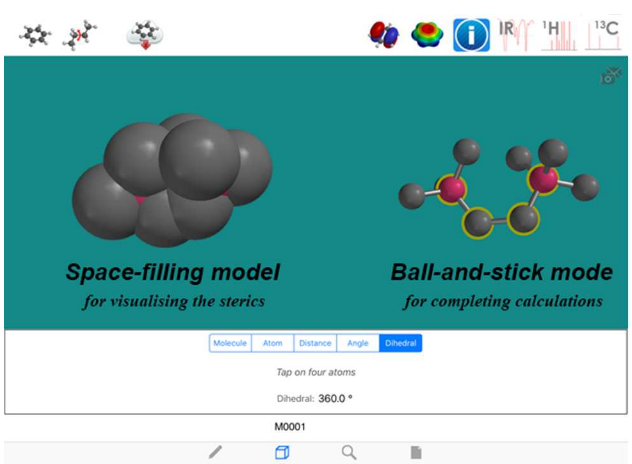

Figure 2. iSpartan screen showing models and measurements generated in Part 4.

Assessment of the Activity

This work was approved by the Institutional Review Board (IRB) at Spelman College. Participants were provided informed consent. The activity was implemented in 2013 and has been completed by four cohorts of students (one cohort per year, average cohort size 20 – 25 students, 92 students total). Assessment data was collected for cohorts in years 2013 – 2016.

Students' gains in knowledge were assessed by comparing the answers to two problems from a pre-assessment, given at the beginning of the semester, and the same problems included on the 1-hour exam administered following the completion of the iSpartan activity. The questions selected represent basic fundamental knowledge and comprehension related to conformations: 1) the ability to interpret Newman Projections by defining the angle between substituents on adjacent carbons and 2) the ability to predict the conformation energy and stability. A total of 84 students responded to both the pre- and post-test questions on interpreting and determining the relative stability of alkane conformations. Outcomes were evaluated by comparing the pre- and post-test scores on questions relevant to the iSpartan activity using two paired samples t-tests. In regards to students' ability to interpret Newman Projections, students performed better after completing the iSpartan activities (post, M = 0.93, SEM = 0.02) in comparison to their performance before the activity (pre, M = 0.33, SEM = 0.05), $t(83) = 10.66$, $p<0.001$. Likewise, students post-performance on the item relating to predicting the relative stability of alkane conformations was improved with respect to that of their pre-performance (average performance post = 0.70, SEM = 0.05; average performance pre, M = 0.14, SEM = 0.04), $t(70) = 8.38$, $p<0.001$.

A survey and post-exam reflection were used to identify students' perceptions of the iSpartan activity and the perceived usefulness of the technology in the course. The survey contained Likert questions, free responses, and multiple choice questions. Of the 58 students responding to the post-exam reflection, 29% indicated iSpartan benefited them the most over that of the other options provided. When asked to indicate the value of using technology for visualizing the conformation and stereochemistry of organic molecules (iSpartan), 71% indicated that it was valuable or extremely valuable. Seventy-nine percent of respondents indicated that iPads/iSpartan should be used in future courses to illustrate conformations, stereochemistry, and mechanisms, with 59% of these indicating the degree to which technology is used for this purpose should be increased. In addition, 63% of respondents agreed with the statement that technology had enhanced their learning. Finally, 57% of respondents felt that iSpartan had enhanced the professor's instruction of the material. Fourteen percent of respondents favored in-class discussion, which during this period consisted primarily of the iSpartan activities. The data suggest that students found the activity and the use of technology in general to be instrumental in their ability to understand and master the topic. In addition, the responses suggest that the iSpartan app should be used to develop similar activities for other structure-based concepts (e.g., mechanisms). In light of this, it is believed that students having access to the app outside of class could potentially increase the benefit of the technology and improve students' understanding of properties that can be correlated to the structure of a molecule.

CONCLUSION

Capitalizing on pedagogical trends, an iSpartan-enabled activity was developed to complement student-centered instruction in the Organic Chemistry I course. The multi-class activity, introduced in Fall 2013, was created to introduce alkane conformations and substituent interactions. By allowing students to utilize the app to identify anti and staggered conformations, students were able to view structural information and connect it to the appropriate terminology. The activity also allowed students to observe the change in physical properties as they manipulated three-dimensional structures. In this way, students were able to generate data and utilize the information to define traditional concepts related to the dynamic nature of alkane conformations. Students' responses to the survey suggest that the activity was instrumental in their ability to comprehend the structural properties related to alkane conformations. This perceived benefit has been reported by other researchers as well.[16, 22] Students demonstrated significant improvement in their ability to respond to questions related to alkane conformations, suggesting concept mastery.

SUPPLEMENTAL INFORMATION

- Instructor's Notes
- Online Assignment
- Example Mnemonic
- Worksheets

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The authors declare no competing financial interest.

ACKNOWLEDGEMENTS

This work has been funded in part by the National Science Foundation HBCU-UP Targeted Infusion Project Award No. HRD-1332575 and the Spelman College Teaching Research and Resources Center.

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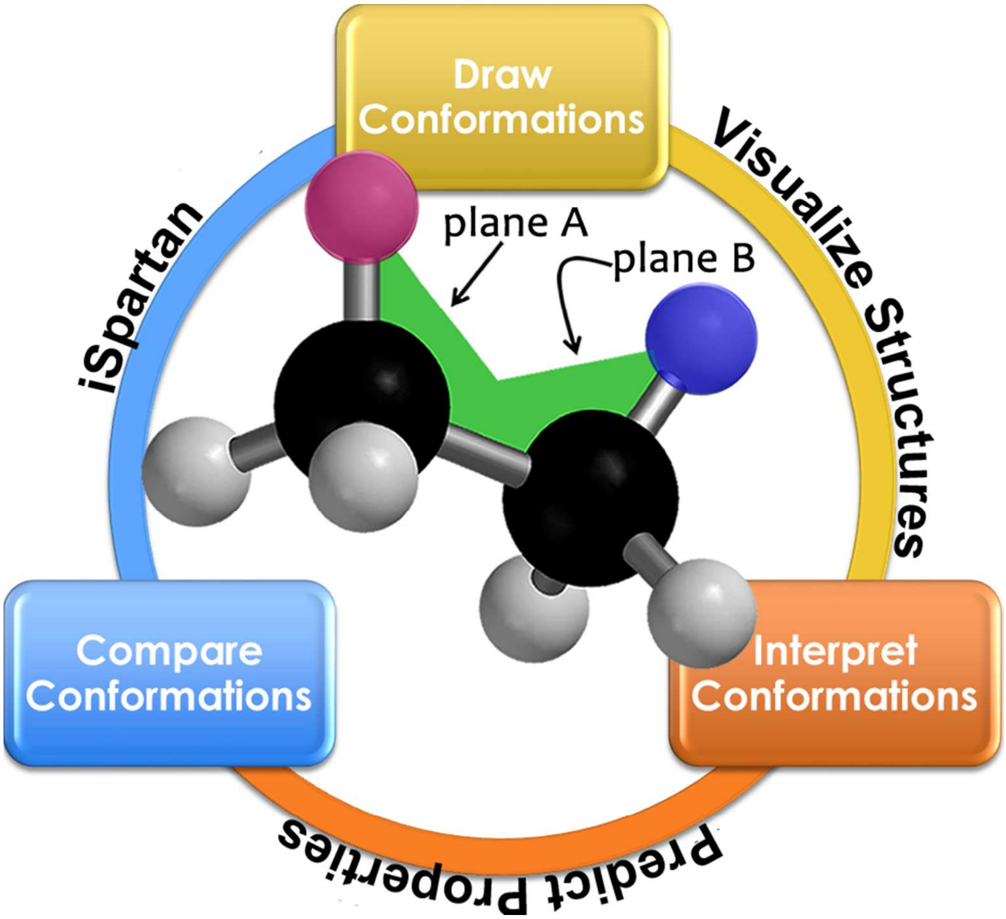

Graphical Abstract

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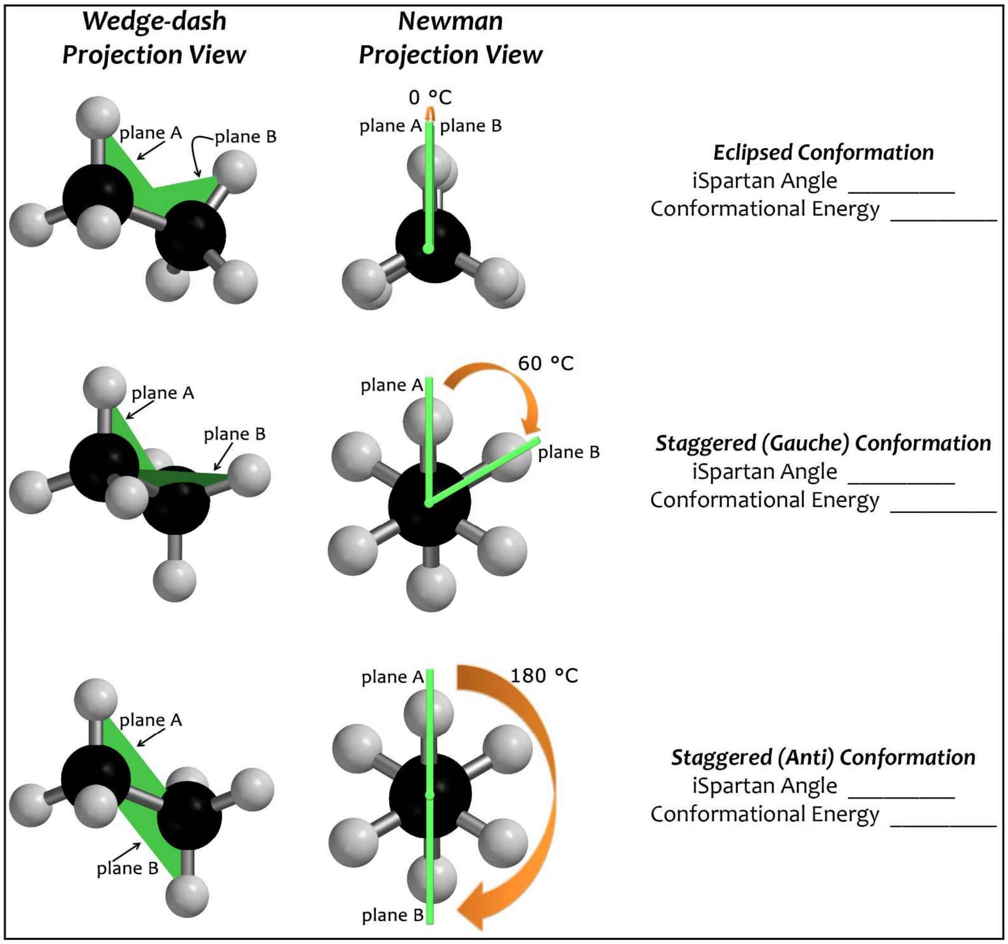

Figure 1

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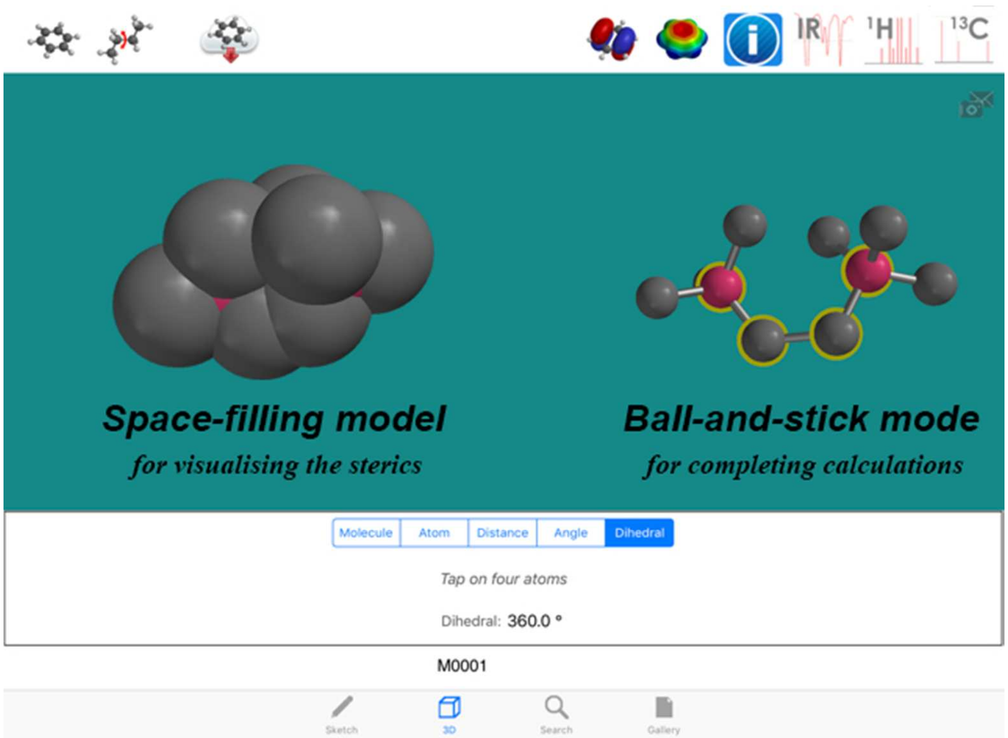

Figure 2

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