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Open-Source Laser-Cut-Model Kits for the Teaching of Molecular Geometry

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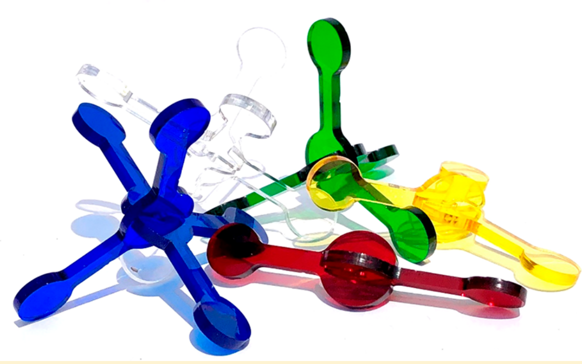
Supporting Information

ABSTRACT: Comprehension of the 3D structure of objects usually represented in 2D is a critical part of understanding molecular geometries. The frequency with which students actually get hands-on with 3D molecular structures is often limited to a singular laboratory session. We sought to develop a set of molecular shapes that were inexpensive enough not only to deploy in a first-year laboratory setting but also to allow the students to take the set home with them to study at their leisure. Laser-cut acrylic parts in five colors were used, and each set could be quickly assembled into the 13 different molecular shapes commonly encountered at the first-year level. The set of shapes was attractive, useful, and easy and fast to fabricate, and they were appreciated by our students. All files have been released in an open-source format, so any interested parties can deploy these models as soon as they secure access to a suitable laser cutter.



KEYWORDS: *VSEPR Theory, Elementary/Middle School Science, High School/Introductory Chemistry, First-Year Undergraduate/General, Demonstrations, Laboratory Instruction, Hands-On Learning/Manipulatives, Laboratory Equipment/Apparatus*

INTRODUCTION

Richard Zare describes chemists as "highly visual people who want to 'see' chemistry and to picture molecules and how chemical transformations happen".[1] At a molecular level, chemical phenomena are often imperceptible; however, experienced chemists have the ability to picture chemistry in their minds by visualizing molecules and their interactions. Although chemists are able to think about molecules in three dimensions, they rely on a variety of visual−spatial representations, such as structural diagrams or reaction equations, to communicate their ideas and teach concepts. As representations are fundamental to discourse in chemistry, representational competence has been identified as a crucial contributor to success within the field.[2] Stieff et al. describe the term "representational competence" as a "discrete set of skills for constructing, selecting, interpreting, and using disciplinary representations for communicating, learning, or problem solving."[3] It is the set of skills that, for example, allows an experienced chemist to spatially interpret a molecular structure and predict reactivity. Research in science and chemical education highlights the importance of representational competency for learning a wide range of concepts taught in general chemistry, organic chemistry, inorganic chemistry, group theory, and biochemistry.[4] Some of the most fundamental concepts and theories taught to undergraduate chemistry students require them to generate, interpret, and fluently translate among a variety of spatial representations. These are tasks that novice chemists often find to be very challenging,[5] and because these skills are heavily relied upon throughout their degree, it may be one of the most significant conceptual hurdles for budding chemists to overcome.[6]

Activities that incorporate the use of molecular-modeling tools, both virtual and concrete, are a common strategy utilized to improve students' representational competence and teach concepts for which the visualization of three-dimensional (3D) objects is necessary. One popular and long-standing version of the concrete model is the conventional ball-and-stick-model kit, often required in first- and second-year chemistry courses. There are many commercial molecular models available, and although they are considered to be highly resilient and powerful, none are inexpensive enough that they can be distributed to the students without making a significant adjustment in the cost of resources. Partly as a result of the cost and also because of questions of scale, creative educators have also built physical models out of a range of media, including coffee stirrers,[7] beads and pipe cleaners,[8] ping-pong balls,[9] Styrofoam balls,[10] whiteboard markers,[11] and circular magnets.[12] As many of these examples utilize inexpensive materials, they are often a cost-effective way to construct one-off models. However, extrapolating them to the size of a large first-year class is not trivial in most cases, and we

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went looking for ways of getting models into the hands of the students not just for the few hours of the laboratory class but beyond.

Previously, we reported the application of hand-held 3D-printing pens to the teaching of VSEPR theory,[13] where students could "draw" and assemble the 3D molecules themselves (other 3D-printed approaches to molecular models are also available).[14] Although these pens were fun to use and created visually attractive molecular models, we found that the pens were slow and unreliable and had a learning curve associated with accurately manipulating the pen. To help facilitate the process of creating models using 3D-printing pens, we provided students with two-dimensional (2D) templates which they could then use to trace all the 2D pieces required to construct the 3D versions of the 13 VSEPR shapes. However, when we trialed the activity with a small group of students working in pairs, we found that each pair only managed to construct a single good-quality model over the course of their first hour, even with the help of 2D templates to get them started, making the technology difficult to deploy in an undergraduate-laboratory setting. We realized that the 2D templates we had constructed to help these students could be deployed in another context, and we decided instead to cut the pieces out of transparent acrylic plastic using a laser cutter (Figure 1). This resulted in perfectly cut, attractive models that snap together in seconds and are inexpensive enough that the students not only can construct them in the lab but can also take them home for use as study aids.

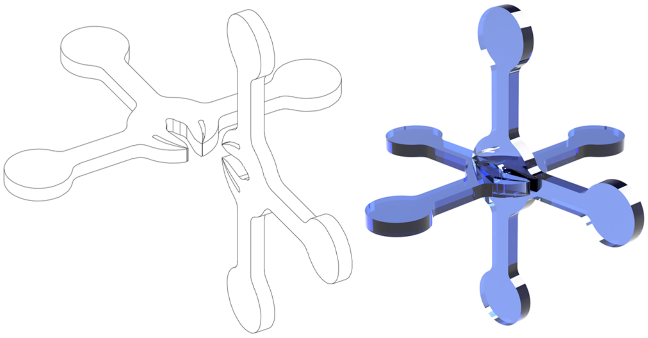

Figure 1. Drawing showing two identical pieces (left) and rendering of the two pieces after they were joined together to form the press-fit model (right).

■ METHODS

Model Kits

The 2D shapes (Figure 1) were laser-cut from colored, transparent acrylic plastic (3 mm cast acrylic, purchased in 4 × 8′ sheets and cut to the bed size of the laser cutter) using a Trotec 130 W Speedy 360 laser cutter. The pieces were designed with slits on either side of the main notch, which allowed for variance in material thickness, ensuring snug fits between the pieces so that the models held together firmly but could also be easily dismantled. The plastic pieces were designed to be interlocked, so that the students could combine the appropriate 2D pieces into the corresponding molecular shape. Each kit contained 26 acrylic pieces, color-coded by the number of electron domains, that could be assembled into 13 molecular shapes (Figure 2). The approximate material cost was $2 per kit. For those using a different bed size, the cut file will have to be slightly adapted (i.e., by deleting excess profiles or cutting and pasting in additional ones). The cut file has been nested as carefully as possible to maximize material usage.

3D-Printed Versions

3D printing is nicely suited to small-scale deployment of these models (e.g., making a single set for personal use). Accordingly, we have provided STL files (a standard 3D-printing format), so these models can also be easily printed out at whatever scale is desired. The default is the same as the laser-cut scale, but because the thickness of the material will scale along with the other dimensions, any size will work.

Surveys

To get a better understanding as to whether the models are effective tools for enhancing student spatial abilities and increasing comprehension of molecular geometry, we created surveys for Chemistry 101 students to complete before and after their laboratory exercise in which they used the models. The first survey came after they had learned the material in class but before they experienced the models hands-on. We created two similar versions of the survey, Version A and Version B (Figures S1 and S2), each consisting of four questions and primarily designed to evaluate student representational-translation ability, which requires students to recognize key features of molecular structures when pictured in unfamiliar geometries, such as in the example shown in Figure 3.

At the start of the laboratory session, half of the students were asked to complete Version A of the survey, and the other half were asked to complete Version B. At the end of the laboratory session, those students who completed Version A were asked to complete Version B, and the Version B students were asked to complete Version A. Although the two versions of the survey were similar in nature, we alternated the versions in this manner to eliminate any potential bias if one of the survey versions was more difficult than the other.

■ DISCUSSION

The deployment and assessment of these models occurred over a 3 year period starting in the fall semester of 2015, which coincided with a major renovation of our first-year chemistry laboratories. This disruption was problematic for us in fairly assessing the efficacy of our new approach relative to the original method, but it did also grant us considerable flexibility in delivering the exercise both in the lab and as a take-home assignment in lieu of a lab (in the term when the laboratory had limited availability due to renovations).

In year 1, no changes were made to the original laboratory exercise, in which Chemistry 101 students were asked to construct a series of molecular models using a combination of polystyrene balls (atoms), toothpicks (bonding pairs), and bent pipe cleaners (lone pairs), as we wanted to acquire control data to compare with our new methodology. In year 2, we replaced the Styrofoam-ball kits with the laser-cut-acrylic-model sets (the current version of this laboratory is contained in the Supporting Information). We surveyed both groups of students before and after the laboratory exercise, and we found that in either case, the average assessment score did not change significantly ($p > 0.05$) after completing the laboratory exercise using the corresponding methods (see the Supporting Information for a summary of descriptive statistics).

The lack of a significant improvement in performance in either the control or in the new lab was somewhat puzzling but perhaps partly a function of the requirements set by the human-research-ethics board at the university: student participation

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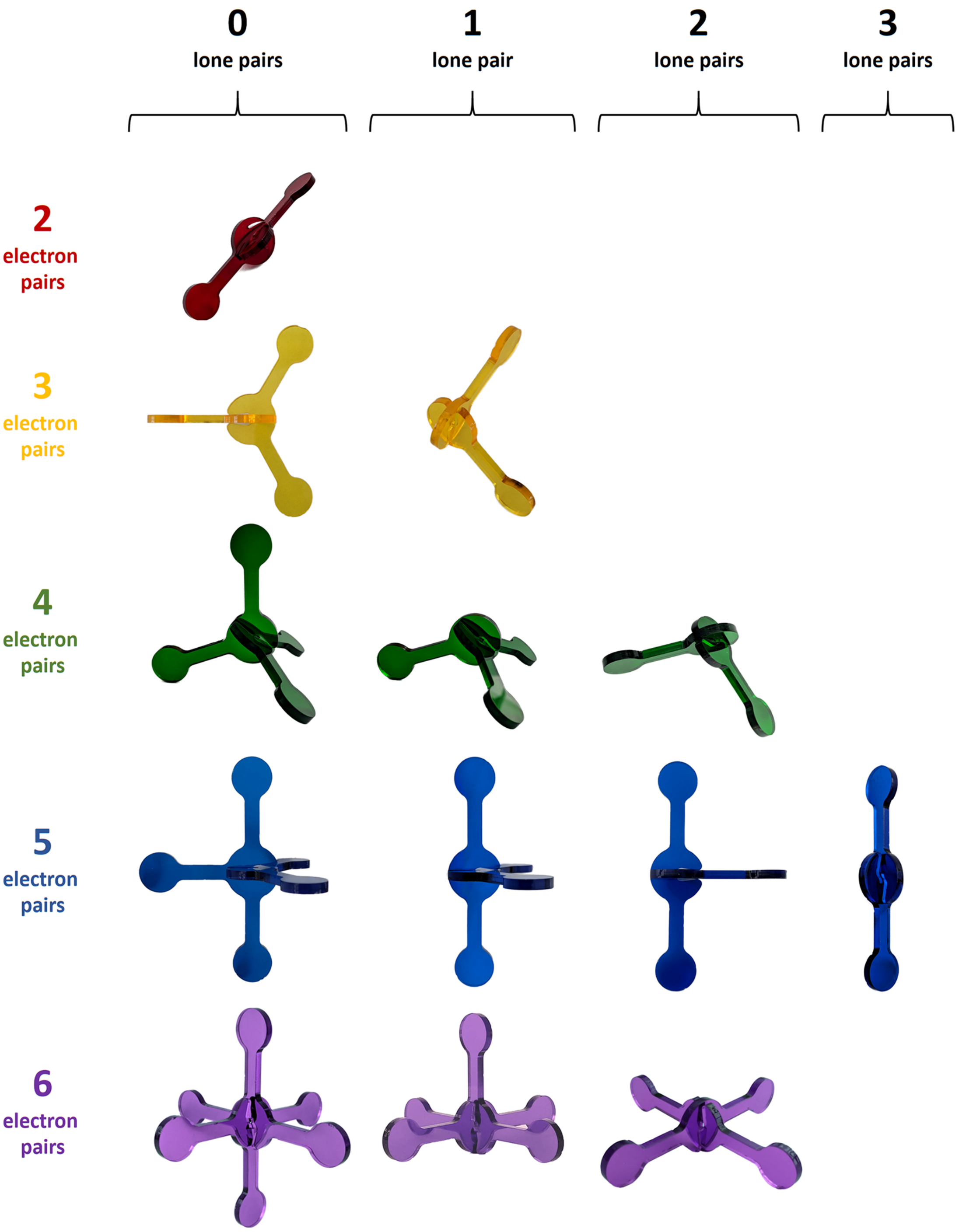

Figure 2. Complete set of laser-cut acrylic pieces, color coded by number of electron domains (nED). (a) Red (2ED): linear. (b) Yellow (3ED): trigonal planar, bent (120°). (c) Green (4ED): tetrahedral, trigonal pyramidal, bent (109.5°). (d) Blue (5ED): trigonal bipyramidal, seesaw, T-shaped, linear. (e) Purple (6ED): octahedral, square pyramidal, square planar.

must be voluntary and as a result of this we found that when students were asked to complete the second, end-of-class survey as they were leaving the laboratory, the participation was not only reduced but often perfunctory. Students were keen to go home or to their next class, which resulted in a large number of students either choosing not to do the survey or rushing through it and not devoting significant thought to their answers. We determined that a better method of surveying was necessary in which students did not feel disadvantaged by choosing to participate in the survey, and an opportunity arose to do so in year 3. Laboratory-availability issues meant all students did the laboratory class instead as a take-home exercise with the material supported by an in-class lecture for which the students brought along their model kits. We were better able to survey reproducibly (using anonymized iClickers in class with fixed time limits) under these conditions, and the before and after results showed a significant improvement in scores ($p < 0.001$), with students scoring on average 9.7% better after completing the laboratory exercise, indicating that these models are most likely effective tools for enhancing student spatial abilities and increasing comprehension of molecular geometry.

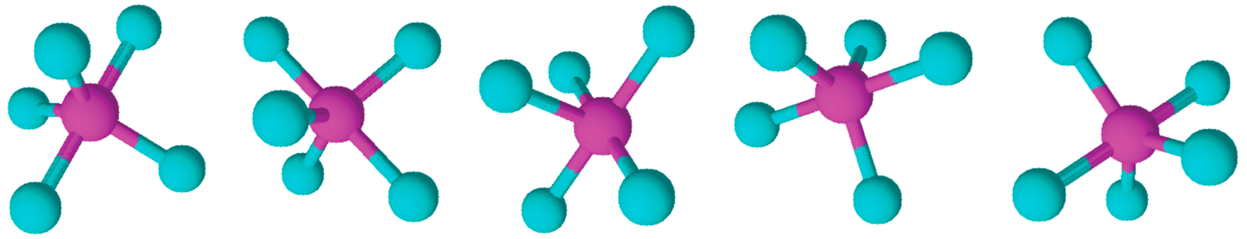

Figure 3. Example question from one of the surveys in which students were asked, “Of the following three-dimensional structures, which represents a molecular geometry that is different from the others?” The third structure is a square pyramid; the rest are trigonal bipyramids. See the Supporting Information for the full surveys (Figures S1 and S2).

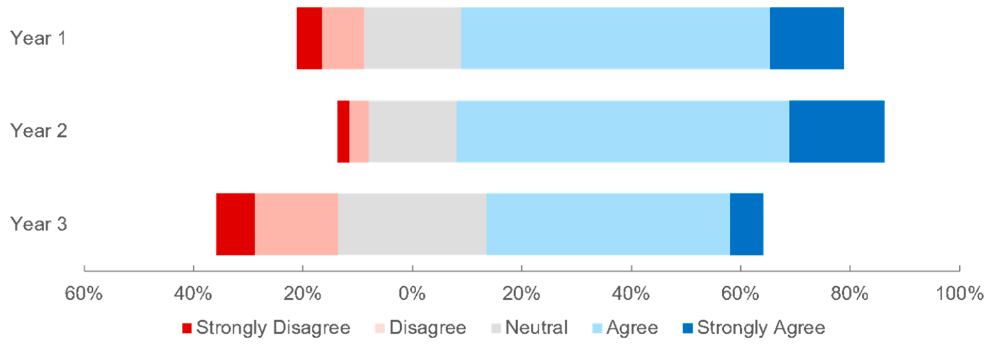

Figure 4. Response distribution for “I learned a lot about molecular shape in this laboratory class/take-home exercise”.

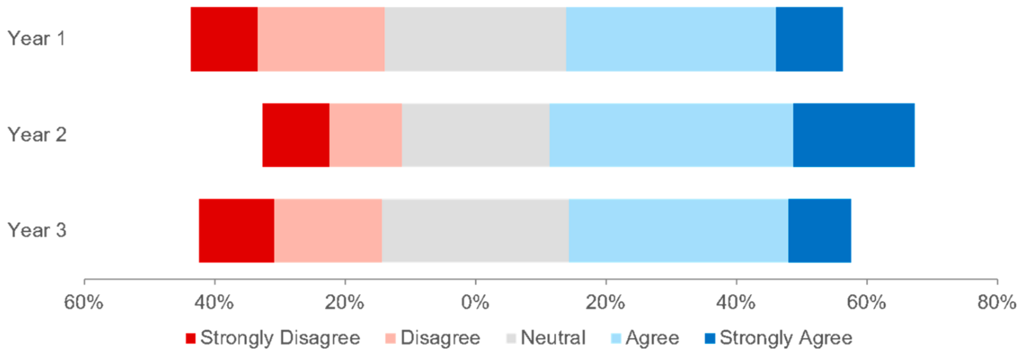

Figure 5. Response distribution for “I enjoyed this laboratory class/take-home exercise”.

We also assessed the students’ *qualitative* impressions of the lab exercise (see the Supporting Information). We asked them to indicate their degree of agreement with two statements: “I learned a lot about molecular shape in this laboratory” and “I enjoyed this laboratory class”. The responses were mixed. When the experiment was run as an actual laboratory class, students generally agreed they had learned a lot (Figure 4), but in year 3, when the laboratory was a take-home exercise supported by a single 1 h lecture, there was little consensus. As far as enjoyment went, results were skewed slightly positive in all 3 years (Figure 5).

CONCLUSIONS

The open-source molecular designs presented here provide an opportunity for educators to enable students to get hands-on with inexpensive 3D representations of basic geometries. Students responded positively to the permanent provision of the 3D models they were taught about in their first-year class. The laser-cut acrylic pieces used were inexpensive enough that they could be given to the students to take home after class, providing them with an enduring reminder of the spatial concepts they were taught in the class and laboratory.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.8b00553.

- Survey used with the statistical analysis (PDF, DOCX)
- Experiment background and procedure information for students, making use of the models described in the paper (PDF)
- Laser-cutting (DXF) and 3D-printing (STL) files used in the construction of the models (the nested files are the ones used for large-scale production of the molecular models and are designed for a laser cutter with bed dimensions of 800 × 500 mm) (ZIP)

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Notes

The authors declare no competing financial interest.

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■ DEDICATION

Our beloved colleague and coauthor Corrina Ewan passed away suddenly in June 2018, just as we were preparing the final draft of this manuscript. This paper is dedicated to Corrina's memory; she was a passionate advocate of science and a wonderful co-worker who will be sorely missed.

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