New visualization tools for learning molecular symmetry: a preliminary evaluation

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Abstract: A Website that helps students visualize and locate symmetry elements on three-dimensional molecular structures was developed. It includes textual explanations, an interactive example window and a Microsoft-Excel based symmetry toolkit that enables students to draw symmetry elements in three dimensions. Preliminary qualitative research aimed at exploring how students learned with this tool was performed. It was found that the three-dimensional graphical capabilities of the toolkit (1) helped students overcome difficulties in three-dimensional visualization, (2) enabled students to find symmetry elements of complex molecules generally not accessible from drawings and (3) contributed to a deeper understanding of molecular structure and chemical symmetry. [*Chem. Educ. Res. Pract.*, 2007, **8** (1), 61-72]

Keywords: Molecular visualization, spatial ability, molecular symmetry, point-group symmetry operations, Web based learning.

Introduction

Molecular visualization is playing a central role in science education in general and in chemistry education in particular (Mathewson, 1999; Jones, Jordan and Stillings, 2001, 2005; José and Wiliamson, 2005). In a recent review, Wu and Shah (2004) summarized the literature regarding visual-spatial thinking in chemistry. They found a positive correlation between students' visual-spatial abilities and their achievements in learning chemistry, in that students with higher visual-spatial abilities performed better than their peers on problem solving in chemistry (both spatial and non-spatial problems). They also pointed out that good three-dimensional (3D) visualization tools (both plastic models and computerized models) enhance students' understanding of molecular structure.

The study of Ferk and Vrtacnik (2003) supports these claims. They investigated how students understand different kinds of molecular representations, and their ability to apply mental operations to molecules. Their findings emphasized the importance of the correct perception of the 3D molecular structure as the basic step preceding any further mental operations. They found that undergraduate university students preferred 3D computerized models or 3D photographs of molecules over other representations (e.g., two-dimensional stereochemical formulas and plastic models). On the other hand, plastic models were more effective for secondary school students.

Molecular symmetry is a topic in chemistry grounded in visualization. It is taught in several undergraduate chemistry courses (e.g., inorganic chemistry, spectroscopy and quantum chemistry) each with its own context and at varying conceptual levels. Understanding the basic concepts of molecular symmetry involves identifying particular symmetry elements of molecules such as rotation axes, reflection planes and inversion points.

To do so requires three skills: (1) the ability to visualize and to understand molecular structures in three-dimensions (spatial visualization), (2) the ability to see and to describe the molecular structure after a rotation, reflection or inversion (spatial orientation skills), and (3) the ability to define precisely the location of symmetry elements in relation to particular atoms. Achieving such conceptual understanding is made harder by the need for students to recognize 3D structures from the static two-dimensional representations found in textbooks. The task becomes even more difficult as the number of atoms per molecule increases and the 3D structure becomes more branched.

A Website entitled "*Molecular Symmetry Online*" that helps students learn molecular symmetry was recently developed at the Open University of Israel by the first author. It includes textual explanations, an interactive example window and a Microsoft-Excel based symmetry toolkit that can be used for drill and practice. The toolkit is an open tool – it enables users to create and draw symmetry elements for *any* molecule in 3D. In this sense it is very different from other recently developed Websites that present symmetry elements within a closed set of molecules (e.g., Korkmaz and Harwood, 2004; Cass and Rzepa, 2005a, 2005b; Charistos et al., 2005).

This study focuses primarily on how students learned while using the symmetry toolkit. A secondary focus was on the capabilities and limits of the tool itself. In what follows, we briefly present the basic concepts of molecular symmetry. We then describe the symmetry toolkit and elaborate on its usage. In the second part of the paper, we describe the findings of preliminary qualitative research performed at the Open University of Israel aimed at exploring how students learned with the toolkit.

Symmetry elements and operations

The symmetry of molecules is described in terms of elements and operations. Elements are geometric entities such as axes, planes and points in space used to define symmetry operations. Operations involve the spatial re-arrangement of atoms in a molecule by rotation about an axis, by reflection through a plane or by inversion through a point. A rotation, reflection or inversion operation will be called a symmetry operation if, and only if, the new spatial arrangement of the atoms in the molecule is *indistinguishable* from the original arrangement. The definitions and applications of symmetry elements and operations are discussed in many textbooks (e.g., Atkins and de Paula, 2006) and will not be repeated here. Table 1 summarizes the symbols of all the possible symmetry elements and operations in molecules.

Table 1. Symmetry elements and operations in molecules.

Symmetry Operation	Symmetry Element	Symbol
Identity	None	E
Rotation about an axis by 360°/n	Axis of order n (proper)	C_n
Reflection through a mirror plane	Plane	σ_h, σ_v, σ_d
Inversion through a point	Point	i
Rotation about an axis by 360°/n followed by reflection through a plane perpendicular to the rotation axis	Axis of order n (improper)	S_n

The *Molecular Symmetry Online* Website

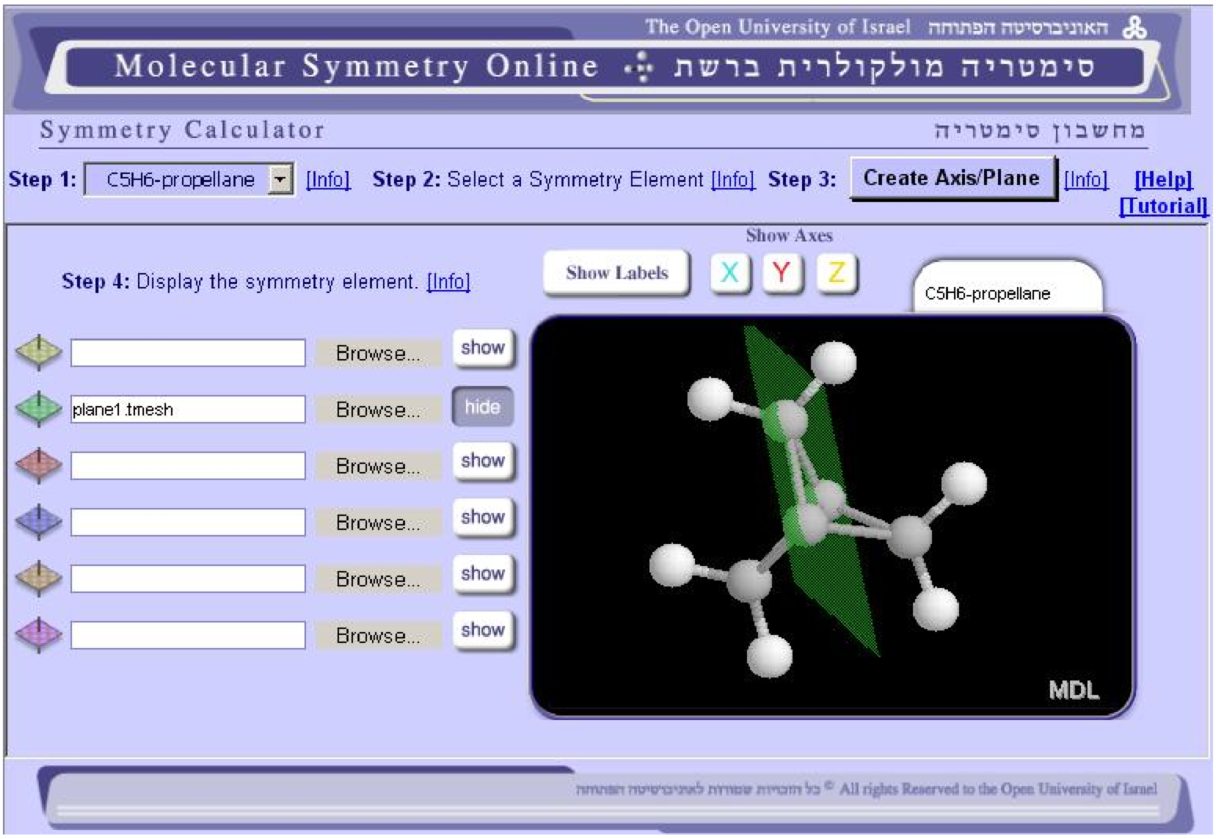
In order to improve visualization of symmetry elements of molecules, and to improve the way students learn symmetry at the Open University of Israel, we recently developed the

Molecular Symmetry Online Website (http://telem.openu.ac.il/symmetry); it comprises two main sections:

- An interactive *example window* presenting six molecules in three-dimensions that users can rotate and translate in space, with or without their symmetry elements. The example window also includes a chemical datasheet for each molecule, a basic tutorial on molecular symmetry and a technical help file.
- The *symmetry toolkit* including a *symmetry calculator* that can be used to create symmetry elements (rotation axes and reflection planes) for any molecule and display them on screen in an interactive, three-dimensional format. The toolkit also includes a database of about 60 molecules, as well as comprehensive didactical and technical help files.

A snapshot of the symmetry calculator is presented in Figure 1.

Figure 1. A snapshot of the symmetry calculator. Working with the calculator is done in four steps. Step 1: loading a molecule from the database, or from the user's computer. Step 2: deciding which element to draw. This is a virtual step. Users can use the 'show label' button to draw the molecule in wireframe with serial numbers on each atom. Step 3: creating the symmetry element using the element and planes wizard. Step 4: loading the symmetry elements created in step 3. Clicking on 'info' at each step opens the relevant help file.



Technology

The Website was built using the Open University of Israel's OPUS system for online courses. The *example window* is a dynamic HTML page in which an MDL-CHIME window is embedded to view molecules in three-dimensions. The *symmetry calculator* is constructed of such an HTML page embedded in Microsoft-Excel and enhanced with a Visual Basic user-friendly interface.

Working with the symmetry calculator is done in 4 steps:

1. **Load a molecule**. The current database contains about 60 molecules, but additional molecules in MDL mol format can be loaded through a browse option.
2. **Decide where to draw a symmetry element**. A virtual step. To define a symmetry element mathematically, the points through which it passes must be specified. Two points in space are used to define a rotation axis. Three points are needed to define a mirror plane. At this stage, inversion points can not be drawn. A point may be defined in one of three ways:
   - a specific atom in a molecule
   - a mid-point between two atoms
   - any point in space

   Atom labels (serial numbers) and Cartesian axes can be displayed in order to help users visualize and specify these points. The molecules in the database were set such that their center of mass is located at the origin. This makes it easier to use the Cartesian axes to define rotation axes that do not go through atoms of the molecule (e.g., C_6 axis in benzene).
3. **Create a symmetry element**. A specially designed 'axes and planes wizard' is used to enter the coordinates of the points in space through which the symmetry element passes. Elements are saved on the user's hard disk. A snapshot of the wizard is shown in Figure 2.
4. **Display the symmetry elements**. Up to six different elements per molecule can be displayed simultaneously. The toolkit displays the elements as defined by the user; it does not evaluate whether the elements are correct or not. Therefore, users can create any element, regardless of it being a symmetry element or not.

Figure 2. A snapshot of the 'axes and planes wizard'. Top: in this screen the user chooses the type of point. Bottom: in this screen the user enters atom types and serial numbers to define a mid point between atoms. The table on the top shows the coordinates of the chosen points.

Usage

The toolkit can be used for drill and practice, testing and classroom presentations. It has been designed as an open tool; therefore it can be used at various content levels and for diverse audiences. Teachers can add molecules to the database thereby allowing students to work on any molecule of interest. Furthermore, teachers may create a solution database so that students can compare their answers with the correct ones. Students may work alone or in groups. The toolkit can also be used for testing purposes. To do so, students submit their calculated symmetry elements for teacher or peer evaluation.

Here are examples for three assignments, based on the symmetry toolkit that can be given to students.

1. Creating symmetry elements of molecules

In this assignment, students are given a list of molecular files for which they need to find part or all of the symmetry elements and draw them on the screen. The complexity of the assignment is a function of several factors:

a. The way symmetry elements are defined
b. The number of symmetry elements in the molecule
c. The spatial complexity of the three-dimensional structure.

The importance of each of the above factors depends on the molecule in question and the student's experience with the symmetry calculator. For example, the water molecule, H_2O, has a very simple planar structure, but defining the reflection plane perpendicular to the molecular plane is a bit tricky since, in the language of the symmetry calculator, it cannot be defined solely by the atoms of the molecule. In contrast, the phosphorous pentachloride molecule, PCl_5, has more atoms and more symmetry elements than water, but these are easily defined in terms of the molecule's atoms. A third example, finding the symmetry elements of urazole, $C_2H_3N_3O_2$ (Figure 3), is more difficult than water, even though they both belong to the same point group (C_{2V}), because the urazole molecule has more atoms than the water molecule and the structure is branched.

For tutoring purposes, we recommend starting with the molecules presented in the example window: CCl_2O, NH_3, N_2F_4, C_3H_4 (allene), PCl_5 and CH_4 (see Figure 4). Although students can see the solutions, locating the symmetry elements and drawing them on the screen is a different task that leads to a deeper understanding of molecular structure. Advanced students can find molecules like twistane (D_2) and Paddle (D_{3h}) quite challenging (see Figure 5, later).

Figure 3. Urazole.

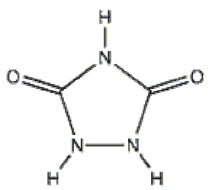
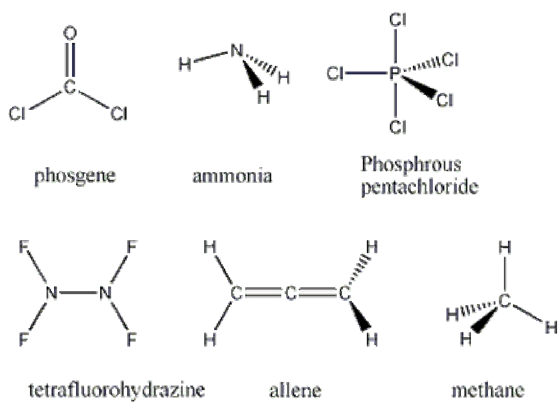


Figure 4. Molecules presented in the example window.



Within the frame of the toolkit, there are several options to provide feedback for the students:

1. Providing files containing the correct symmetry elements. Students can overlay these files onto their own files within the symmetry calculator and see if they match.
2. Providing the answer in the form of the points in space (atoms, midpoints or others) through which each element passes.
3. On-site feedback from a teacher/tutor who watches the student's work.
4. Asynchronous textual feedback from a teacher/tutor.

2. Symmetry Reduction

Another type of assignment involves the analysis of symmetry after substitutions. For this purpose, the teacher should prepare a series of molecules where one or more of the atoms are substituted by other groups. Planar structures like aromatic cyclic molecules or crown ethers are good examples, but more complex structures can be used for advanced students. One can start with benzene, for example, and ask students to find all of its symmetry elements. In the next step, the students are given chlorine derivatives of benzene. Students should then decide which of the symmetry elements of benzene remain symmetry elements for each derivative. For this purpose, they do not need to redraw the elements, just overlay them on each derivative.

3. Defining the location of symmetry elements

In this assignment, the teacher prepares in advance files of elements for a number of molecules. The students then need to decide whether these elements are symmetry elements for the listed molecules, and describe the location of these elements, either in words, or by creating their own elements to match the teacher's elements.

The current study

Background

The Open University of Israel is a distance education university designed to offer academic studies to students throughout Israel. Established in 1974, the university offers a home study system based on textbooks, instructors, face-to-face tutorials and course Websites. The university offers a variety of programs for both bachelor and master degrees. Enrollment for the academic year 2004-2005 was about 40,000 students. As course study loads are relatively high, most students register for only two or three courses per semester; most do not complete any degree program. On average, it takes about seven years to finish a bachelor's degree.

The course, inorganic chemistry, from which students volunteered to participate in the study, is an intermediate level course required for all chemistry majors. It accounts for 6 credits out of a total 108 needed for graduation. The course material includes 12 self-study text units, based on Shriver and Atkins' (1999) *Inorganic Chemistry* textbook. The second unit deals with molecular symmetry. Molecules and their symmetry elements are presented in this unit by two-dimensional drawings. As part of the learning materials, students receive kits (plastic balls and sticks) that are used to build three-dimensional models of molecules. There are six face-to-face tutorial sessions during the semester in which students may participate. Participation is not obligatory. The first session is devoted to molecular symmetry. In addition, students submit written assignments during the course. The first assignment includes problems in molecular symmetry.

Research Rationale and Objective

After an extensive literature review, no previous studies were found that tested the way students learn molecular symmetry using interactive three-dimensional representations of molecules and symmetry elements. Initial investigations into a phenomenon as subtle and complex as student learning require an in-depth examination of individual learners in order to produce preliminary findings. A grounded theory approach (Glaser and Strauss, 1967; Glaser, 1978; Cohen and Manion, 1989; Charmaz, 1995; Strauss and Corbin, 1998) generally begins with small naturalistic studies carried out in order to generate models and hypotheses that can then be tested on larger populations using traditional statistical techniques.

Based on these assumptions, a small naturalistic study was planned and carried out. Objectives were twofold. First, to describe how students learn molecular symmetry by means of the Website's features (the interactive example window and the symmetry toolkit), and second, to judge their perceived effectiveness in relation to the two-dimensional methods used during the course.

Participants

18 students enrolled in the course 'Inorganic Chemistry' during the spring semester of 2004. All students were offered the opportunity to participate in the study. Six chose to do so (five men and one woman). All students who took part in the study had previously completed the course 'General Chemistry' which is a prerequisite for registration in 'Inorganic Chemistry'. They were, therefore, experienced in distance learning at the Open University. All students submitted the assignments on molecular symmetry and received passing grades (above 75 on a scale from 0 to 100). The average grade was 87. The average grade of the whole class was similar (10 out of 18 students submitted this assignment).

Interviews with students

Students participating in the study were invited to a personal interview/tutorial session that lasted between 90-120 minutes. Interviews/tutorials were carried out by both authors who were in no way directly related to the course. This was emphasized so that students would not be reticent or apprehensive about offering information freely. Complete confidentiality was assured. The interviewers did not know any of the participating students. Sessions took place towards the end of the semester, prior to the final exam and about two months after the students had completed the second unit of the course which dealt with symmetry. From the students' point of view, these sessions were an opportunity to have a private lesson prior to the final exam.

All sessions were tape-recorded. During the session, one interviewer made brief notes; immediately upon its completion, both interviewers made extensive notes. The interview/tutorial had four parts: (1) preliminary discussion, (2) pretest, (3) instructional session and (4) summation.

The preliminary discussion was intended to create a friendly and open environment. Students were told about the study and its goals. They spoke about themselves, their studies, goals, future plans, etc.

The pretest included the following questions about basic symmetry concepts:

- What is a rotation axis? Draw an example.
- What is a reflection plane? Draw an example.

Students were also asked to find the symmetry elements of water and methane. These molecules were chosen on the basis that students were familiar with their symmetry, since they were previously discussed in the course. For each molecule they were asked to:

- Draw the molecule and all of its symmetry elements.
- Describe verbally the spatial location of the symmetry elements.

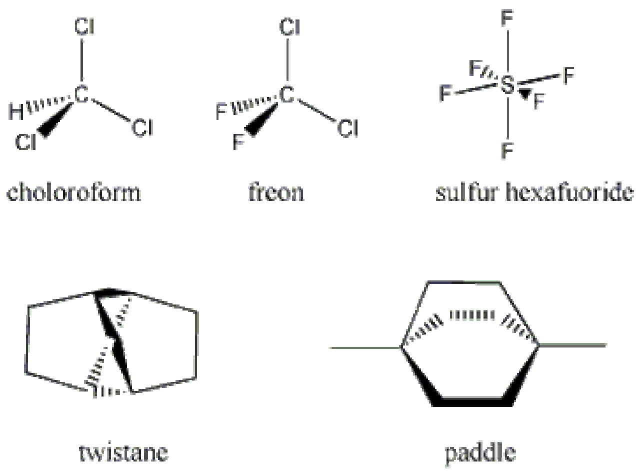
- Draw the molecule before and after specific symmetry operations by assigning serial numbers to the atoms.

Students were expected to answer these questions on paper, and/or orally. Plastic models were not provided.

The instructional session included:

- An introduction to the symmetry toolkit by using the “example window” where they could see the symmetry elements of methane in interactive 3D format.
- A short demonstration of how to use the symmetry calculator, during which the symmetry elements of the water molecule were drawn on screen.
- A work session in which students were asked to find symmetry elements of molecules by using the symmetry calculator. The set of molecules included: chloroform, Freon, paddle, twistane, and sulfur hexafluoride. These molecules are shown in Figure 5.

Figure 5. The set of molecules included in the instructional session.



The summation included questions about students’ use of the toolkit, especially how they learned and their evaluation of its effectiveness.

Results

Preliminary discussion

Preliminary discussion created a friendly and open environment for all participants. Students spoke freely, and any initial unease or tension about being questioned and judged quickly dissipated. Students viewed the session as a tutorial aimed to help them understand symmetry concepts which, at the same time, aimed to help us understand the learning process.

Pretest results

All students were able to identify the symmetry elements of water (however, 2 out of 6 had problems with one of the reflection planes). Most of them failed to see all the symmetry elements of methane. Since the C_3 axes of methane overlay with the C-H chemical bonds, these were easily identified by all students. However, only one student identified the C_2 axes that are located between the bonds. The reflection planes were identified partially by four students, fully by one student and not identified at all by a sixth student. Table 2 summarizes the pretest findings. For the sake of privacy, students’ names were changed.

Table 2. Students' spatial abilities prior to working with toolkit.

Molecule →	H_2O			CH_4		
Element → **Name ↓**	C_2	σ_v	σ_v'	$3C_2(=S_4)$	$4C_3$	$6\sigma_d$
Oren	Yes	Yes	No	0/3	4/4	3/6
Moshe	Yes	Yes	Yes	0/3	4/4	3/6
Danny	Yes	Yes	Yes	0/3*	4/4	3/6
Jacob	Yes	Yes	Yes	0/3	4/4	1/6**
Hanna	Yes	Yes	Yes***	0/3	1/3**	No
David	Yes	Yes	Yes	3/3	4/4	6/6

Instructional sessions and summations

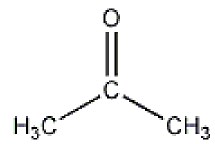
All students were introduced to the Website by using the 'example window' where they could see the symmetry elements of methane in interactive 3D format. This was followed by a short demonstration of how to use the 'toolkit', during which the symmetry elements of the water molecule were drawn on screen. All students readily grasped the toolkit's methodology for drawing symmetry elements; that is, using atoms, midpoints between atoms and any point in space to define axes and planes. In what follows we describe in detail the work session of four students.

Moshe dealt with the first molecule presented, chloroform, by creating his own mental image of the molecule from the diagram in order to identify the symmetry elements. He began with reflection planes and found all of them, without using the symmetry toolkit. Moshe reported that he was able to visualize the model in his own mind and see the symmetry elements clearly. Immediately afterwards, he replicated the same task, this time using the toolkit. He easily identified and drew the symmetry elements. The 3D representations enabled him to confirm that his mental images were indeed correct. He said: "*I can see the symmetry element in my mind, but I'd rather use the toolkit to draw it and check if I'm right.*"

Next, Moshe chose to work on acetone (CH_3COCH_3, see Figure 6). Although this molecule was not on the list of molecules we intended to examine, we allowed him to continue. He created his own mental image of the molecule from the diagram but failed to identify the symmetry elements. Using the toolkit, however, he was able to identify all the rotation axes and reflection planes. For the following two molecules, paddle and twistane, Moshe made no attempt to create his own mental images (the molecules were too complex) and began directly with the toolkit. For both molecules, he identified the rotation axes. He also identified some of the reflection planes of paddle.

To conclude, Moshe pointed out that the toolkit enabled him to skip the critical step of internal visualization. Since the toolkit enabled him to view the three dimensional structure directly, he could concentrate on finding symmetry elements. Using the toolkit, he was able to find elements that otherwise would not have been found.

Figure 6. Acetone.



Danny used only the toolkit to find all the symmetry elements for the following molecules: $CHCl_3$, CCl_2F_2, Paddle, SF_6, and Twistane. He did not draw the symmetry elements on the screen since he was able to identify the symmetry elements with a high degree of certainty just by viewing the 3D molecular structure. He found the ‘axes and planes wizard’ of the toolkit “*tedious and time consuming*”. Danny reported that, although he was capable of imagining simple 3D structures in his mind, he preferred to work directly from the screen without any internal visualization. He said: “*I no longer need to imagine the structure in my mind*.”

Hanna was incapable of visualizing any three dimensional molecular structures from their drawings on paper. This limitation severely handicapped her understanding of the basic concepts of symmetry. She was unable to define rotation axes and reflection planes since she had no language through which she could do so. She was unable to draw any molecule except HCl.

In order to proceed, Hanna was reintroduced to the concepts of symmetry by using the ‘example window’. She was then introduced to the toolkit. Together with the researcher, she worked on two molecules, water and methane, for about twenty minutes. Upon completion, she was able to define and to identify rotation axes and mirror planes. She said: “*Before I couldn’t see anything. Now I do*.”

Next, she worked alone on two molecules, chloroform and Freon. She was able to identify rotation axes and mirror planes in both. She was extremely excited, even thrilled, at her new found visualization skills. Despite the two hour length of the tutorial session, Hanna wanted to continue and work on additional molecules. The authors politely declined.

David used the toolkit to find *all* the symmetry elements for the following molecules: Freon, Paddle and Twistane. For the first two molecules, he did so quickly and easily, claiming that the 3D visualization is not really essential since he can visualize them in his mind. However, he noted that the 3D representations of the supposed symmetry elements helped him to decide if, in fact, they were correct. For the twistane molecule, he worked confidently, but required more time to complete the tasks. He said: “*The toolkit really helps here because I can’t visualize this molecule at all without it*”.

Concluding Remarks

The Website’s primary features, the ‘example window’ and toolkit, helped students to overcome difficulties in 3D visualization. Even students with good visualization and orientation skills preferred to work with the computer graphics, especially for complex molecules, thereby eliminating the need for the now redundant step of internal visualization. Interviews with the other two students, Oren and Jacob, not described above, support these findings.

Usually, tasks that require finding symmetry elements of molecules rely on student's intuition and drawing capabilities. Questions of this type are usually phrased: “*Find the symmetry element of …*” Students’ answers to such questions are usually given in the form of a drawing, without explanation. The symmetry toolkit provides an alternative didactical way to solve these problems. In order to draw a symmetry element on screen, it must be defined as a geometrical entity, that is, the points in space through which it passes must be specified. In our opinion, solving the task in this way contributes to a deeper understanding of the basic concepts of symmetry, as was seen in the case of Hanna described above. She represents an extreme example of a student with difficulties in spatial ability. The toolkit not only helped her understand the three-dimensional structure of molecules – it also provided her with a language to solve problems. Nevertheless, further research is needed to generalize this finding.

From an instructional point of view, the Website can be used for drill and practice, testing and classroom presentations. It is an ‘open tool’ that provides teachers with an interactive framework to teach the molecular symmetry of any molecule. It can therefore be used for various courses at different levels and for diverse audiences. Further research with this tool is required in order to optimize its use. Some tentative research ideas are: exploring the sequence of molecules that will allow students to learn basic concepts of symmetry with maximal success and minimal frustration; understanding the origin of students' difficulties in finding symmetry elements – spatial visualization, spatial orientation or the ability to define the location of symmetry elements; comparing the way students solve problems on paper before and after working with the toolkit.

From a technological point of view, the major advantage of the Website is its ability to define, save and upload symmetry elements of any molecular structure so desired by teacher, student or researcher. Further avenues of development might include creating an online version of the toolkit; replacing Chime with Jmol (http://jmol.sourceforge.net); adding other features such as solutions for the set of molecules in the database and assigning point groups for these molecules. More sophisticated developments may include applying the method of the continuous symmetry measure (Zabrodsky et al., 1992; 1993) in order to provide an immediate feedback to symmetry elements drawn for any molecule.

The authors will be happy to collaborate in further research and development of the Molecular Symmetry Online Website. Please contact the first author for details.

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