A Review of
3DMolSym (Interactive Molecular Visualization of Symmetry Elements and Operations)
A Web Resource designed and developed by Michael Sigalas and Nicolas Charistos

Several members of the IONiC community (myself included) have posted information on VIPEr about web sites to help students visualize molecular symmetry. I will provide links to each of those found on the VIPEr site. This learning object is to alert you to a wonderful site that has been available for years and has more recently been upgraded so that it can be viewed on a Mac platform as well as the Windows platform it was originally designed for. The 3DMolSym website, designed and developed by Michael Sigalas and Nicolas Charistos, uses Adobe Shockwave Player animations of molecular symmetry elements and operations. The operations can be viewed from any orientation selected by the user, and the speed can be adjusted to accommodate the viewer. Fantastically, the atoms prior to the operation "are ghosted" so that when the operations are complete you can see that symmetrically related atoms return to result in an indistinguishable orientation. When I first saw this site in 2005, I was particularly taken by how wonderfully the S_n operations were animated. (Note: this site was reviewed in J. Chem. Educ. in 2005: Vol 82, p. 1741) For those of you familiar with Dean Johnson's website "A Symmetry Tutorial" you will see many similarities. Dean Johnson's site is scripted in Jmol and JSmol; 3DMolSym uses Shockwave. These are both fantastic Web sites and great teaching tools. I encourage you to check out both of them!

Go to http://www.molwave.com/software/3dmolsym/3dmolsym.htm. On the opening page, go down to "In Summary, with **3DMolSym** you can:" and click on the bolded **3DMolSym** to get started. Alternatively you can go to the bottom of the page and click on **launch 3DMolSym**. Adobe Shockwave Player will begin and then you will be asked to Enter. (Note you may be asked to install a plug-in for Adobe Shockwave Player if it is not loaded onto your computer).

If you are using a Windows machine once you enter, you can select a molecule (of which there are many). Next click on a box to the left of an element/operation to see the symmetry element about which the operation will be performed. To perform the operation, you need to highlight the operation (by clicking to the right of the box on the operation itself). On the left under the molecule you can choose a viewing speed and then click on the arrow to perform the operation. So for example call up "iron hexapyridine", select the S_6, carry out the operation in slow motion and enjoy!

If you are using a Mac, Before you select a molecule, go to the upper right hand corner and change anything in the pull down menu (with Symmetry Elements Selected which is how the resource will open. Under Element Type, select Axes or Planes, or even reselect All Elements). Once you do this, the resource will correctly call up the molecule you select (if you don't do this, the molecules will be frame shifted by one selection, so for example when you select ammonia you will see Adamantane). After you have taken care of this one bothersome flaw, you can return the Element Types to All Elements if you want more choices. Now you can select a molecule (of which there are many). Next click on a box to the left of an element/operation to see the symmetry element about which the operation will be performed. To perform the operation, you need to highlight the operation (by clicking to the right of the box on the operation itself). On the left under the molecule you can choose a viewing speed and then click

on the arrow to perform the operation. So for example call up "iron hexapyridine", select the S_6, carry out the operation in slow motion and enjoy!

Learning goals:

Working with this web-based resource

1. Students should be able to visualize symmetry elements and operations.
2. The beauty of molecular symmetry can be further appreciated with this tool.

Assessment:

To date, I can share only anecdotal evidence that when using web-based tools for visualizing symmetry that students are more capable of assigning point groups. In the past, providing students with models was useful, but in complex models, the molecular symmetry can easily be accidentally altered. I find the web-based materials allow the students to work on the problems until they feel comfortable. They can perform operations from many orientations and benefit from examples provided. I test the students skills with a different site (developed in 2005 and also reviewed in J. Chem. Educ.; Vol 82, p. 1742) : Rzepa and Cass: An Interactive Animated Overview of Molecular Symmetry: http://www.ch.ic.ac.uk/local/symmetry/) that give students some tools for testing rotational axes, but does not give them the point group answer or carry out correct symmetry operations for them.

Links to similar or related Web Resources:

Author: Dean Johnson: "Symmetry Resources at Otterbein University": http://symmetry.otterbein.edu/index.html

Authors: Marion Cass and Henry Rzepa: The Structure and Symmetry of the Metal Tris Chelates: http://www.people.carleton.edu/~mcass/TrisChelates/jsmol/Index.html

Authors: Marion Cass and Henry Rzepa: An Interactive Animated Overview of Molecular Symmetry: http://www.ch.ic.ac.uk/local/symmetry/