photon" when asked to define fluorescence. Although the final answer is a component of the correct answer, it was not a complete answer.

Table 1 Pre/Post Test Results

Classes	**Pretest average score out of 5**	**Posttest average test score out of 5**
Anatomy and Physiology 10 students	1.8	3.5
Chemistry I students with traditional instruction 31 students (2 classes)	2.85	3.4
Chemistry I students without traditional instruction 25 students	2.08	3.2
Chemistry I students with only traditional instruction 24 students	1.25	1.9

All students in the classes tested made improvements from their pretest to the post test scores, which may indicate an increased understanding of what fluorescence is and how it works. Students' answers on the short answer part of the assessment became more in depth and comprehensive. On the pretest, examples of their answers to the question "Define fluorescence." were; blank answers, "a molecular process", "the amount of energy to complete something", "chemical substances made from fluorine", and "I don't know". Of the twenty-five Chemistry I students, twenty-three students were unable to properly define fluorescence. Most students seemed to have no prior knowledge of what fluorescence was before the activity. The activity seemed to improve their understanding of what fluorescence is and what causes compounds to fluoresce. On the posttest, answers to the same question become more in-depth, like "the emission of light after an excited state".

4. DISCUSSION

Research has shown that fluorescence is best understood by looking deeper than just the geometry of a molecule. Although double bonds may be a good reason to look deeper, the possible transitions that cause fluorescence are effected by not only the arrangement of nonbonding and bonding orbitals within the molecule but also the environment such as hydrogen bonding. Moreover because energies are effected by various conditions including the orientation of the p orbitals, the circumstances leading to fluorescence in molecules differ depending on whether the molecule is azoaromatic, or a carbonyl, etc (Sidman, 1958). Because understanding the reasons for fluorescence are so complex students would not be able to reach any clear answer, but should be able to hypothesize some generalities.

Students were able to perform the energy drink activity easily. Most of the students had previous working knowledge of WebMO and the team structure allowed the inexperienced students to complete the lab. The directions were detailed and step-by-step preventing students from making many mistakes. Unfortunately, there was a problem in the procedure for importing molecules that was addressed in the student instructions. The student instructions failed to tell students after importing their second molecule to open the editor in WebMO and select "Cleanup; Comprehensive mechanics" to attach hydrogens where needed. This mistake caused numerous failures of their model runs for several groups, which began to frustrate some of the students until the mistake was found and corrected in the instructions. Students also had trouble building the molecules they were assigned. However, with teacher guidance they were able to rebuild the molecule quickly and complete the lab without incident. It was also observed that once one student was shown how to overcome a technical problem in WebMO, they would help others around them. This helped foster cooperative learning. Overall, the instructions were well written and allowed the activity to be completed in a timely manner.

The data sheet also had its pros and cons. Overall, the data sheet was easy for students to follow and complete. Some students needed clarification with a few of the questions; however, the data sheet was clear and concise. Unfortunately, there was a problem with student understanding in the questions that dealt with the ultraviolet visible absorption graphs. Students consistently missed questions dealing with the ultraviolet visible absorption graphs in the WebMO output and how to interpret them as evidenced in the post test. More time discussing these graphs may have furthered understanding. Also, some students answered some questions incompletely, listing only one similarity between substances. Overall, students were able to perform the activity in an acceptable time with minimal questions. The post test seems to indicate that this experience did allow students to gain knowledge of fluorescence and factors that could perhaps cause it.

In the chemistry 1 class during the post test, out of the twenty-five students, sixteen consistently missed at least one of the two questions that referred to the emission spectrum graph. Even after completing the lab, they were unable to decide if the wavelength or the intensity indicated the visibility of light. They also were unable to distinguish which part of the graph, the intensity or the wavelength, indicated the amount of energy being released. Also, in the laboratory data sheets students only recognized one similarity in either the molecular geometry or the ultraviolet visible absorption spectrum. They were unable to find multiple similarities or find similarities in both the molecular geometry and ultraviolet visible absorption spectrum. Finally, students were unable to draw the conclusion that using only ultraviolet visible absorption and molecular geometry did not give them enough information to determine if a molecule would fluoresce or not. The students tested did not understand that this is a current area of study and a definitive answer is not available. After the post test, the control group of twenty-three students had nine students correctly identify if light was visible on an emission spectra graph. None, however, could identify which part of the graph, the intensity or the wavelength, indicated the amount of energy being released. This showed that the project did allow for further understanding of the energy associated with the emission spectra.

To fix the problems faced in this activity some changes should be implemented. The first clear change would be to add steps in the instructions for importing molecules. We need to clarify that the students should clean-up their molecule to add hydrogen in the needed places for the proper computation to take place. The data from the students supports the idea that this "Ice Cube" is best used as a part B where A is the introductory material for the subject being studied that could include listing and identifying molecular substructures such as carbonyl, nitroso, azo, and other hetero groups as well as aza aromatic compounds or simply recognizing ring structures, double-bonds and alternating bonds. Other introductory material could include experience with optics, the electromagnetic spectrum, light intensity, emissions, wavelength and frequency. Using the data from the students, the activity should be edited to help achieve more understanding of ultraviolet visible absorption and the differences in molecular geometry (J. Sidman, 1958). There should be more introduction and discussion of the ultraviolet visible absorption, and what wavelength can be represented and the visible spectrum. Finally, students should be prompted in the data sheet to look more deeply into similarities in geometry and ultraviolet visible absorption. This activity was designed to illustrate the unknown properties of scientific discovery. Students have very little contact with the unknown in the traditional classroom setup. Very little can be done to improve the frustration of the students in an activity where the outcome or answer is unknown. This can only be eased with more exposure to this type of activity.

Ultimately this activity allowed for the students to be active participants in the scientific method and in learning the complexity of determining a cause for fluorescence. The students were asked to gather information, ask questions, submit a hypothesis, test this hypothesis and discuss the results. They were put into a situation where they were testing a problem without a clear answer. This confused most students but also gave experience in real-world science. The students gained insight on doing research when there is no clear answer. This model, when compared to the control group, showed furthered understanding of this topic and scientific reasoning.

5. CONCLUSION

WebMO allowed students to build complex virtual molecules that they would have difficulty building in the classroom using other modeling techniques, such as ball and stick models. Also, WebMO allowed students to use the molecule they built to find new information about each molecule. Students looked at structure, the molecular geometry as well as ultraviolet/visible absorption in hopes of understanding how these features might affect its fluorescence. From the data collected, using WebMO allowed students to gain a better understanding of the concept of fluorescence. The experiment also allowed students to participate in a lab that would otherwise require some very expensive equipment to find the spectra of the molecules or require the use of literature to find the spectra. The "Ice Cube" allowed them to be active participants in the learning of the scientific method and how complex the topic of fluorescence is. WebMO allowed students to visualize the molecules they studied instead of just looking them up in reference books. WebMO is a powerful tool that allows students to investigate electron density, infrared spectra, NMR and other data. With today's students being more and more technologically savvy, WebMO can be used to help introduce complex topics that are almost impossible to visualize in real life.

Ultimately, this activity did succeed in encouraging and fostering scientific inquiry in the students. The students gained experience in taking real-world occurrences and applying the scientific method to understand the mechanisms behind observations. This activity also allowed the students to apply learned topics in chemistry to their everyday experiences. This activity did improve student understanding. Students, when compared to the control group, had a more in-depth knowledge of fluorescence, molecular structure, graph reading after participating in this activity. Further improvements will make this an even more successful way of introducing these topics.

6. ACKNOWLEDGEMENTS

We express our sincere appreciation to the ICLCS staff and members for their support and encouragement on this paper and the development of this "Ice Cube". We also would like to thank the University of Illinois for the use of their facilities and supercomputers and NSF for their funding of this program.

7. REFERENCES

[1] NIST Chemistry WebBook (2008). *Molecules used for importing*. Retrieved from: http://webbook.nist.gov/chemistry/

[2] Sidman, Jerome W.; Electronic Transitions Due to Nonbonding Electrons in Carbonyl, Aza-aromatic, and Other Compounds; Dept. of Chemistry, Cornell University, Ithaca, New York March 1, 1958