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Projecting Computer Generated 3D Molecular Images in a Chemistry Lecture Hall

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Abstract. Students often have difficulty visualizing the three-dimensionality of chemistry and all that such structural features imply. While chalk-boards, 2D drawing programs, “pseudo” 3D programs, and physical models are effective teaching tools, and used to a greater or lesser extent by most chemistry lecturers, inexpensive computer hardware has made it practical to project true 3D images in large lecture halls. To ease the concerns in designing and installing a 3D projection system for use by chemists, we outline the products we have used and the experiences we have had in upgrading our chemistry lecture hall to be capable of projecting stereo images for 3D visualization. The system described is readily adoptable by everyone and is a turn-key system for detailed projection of any molecule, large or small, as well as showing animated 3D reaction mechanisms.

Introduction

“A picture is worth a thousand words.” This old saying is generally thought to mean that sometimes a picture succinctly captures a complex set of ideas that are difficult to unpack into works. Chemistry textbook authors certainly seem to accept the adage as their books, which are often the first point of contact with students, are filled with pictures and diagrams. Undoubtedly, many chemistry practitioners will agree that chemistry is a visual science in that it relies heavily upon symbolic representations to convey ideas (*1*). However, pictures and diagrams do not always mean the same thing to every viewer. Some of us are simply better visualizers than others. Some pictures have special disciplinary “codes” such that viewers without the requisite training see a pretty picture whereas specialists see explanation and predictive properties. As a case in point, consider a picture of cyclohexane, three renditions of which are shown in Figure 1.

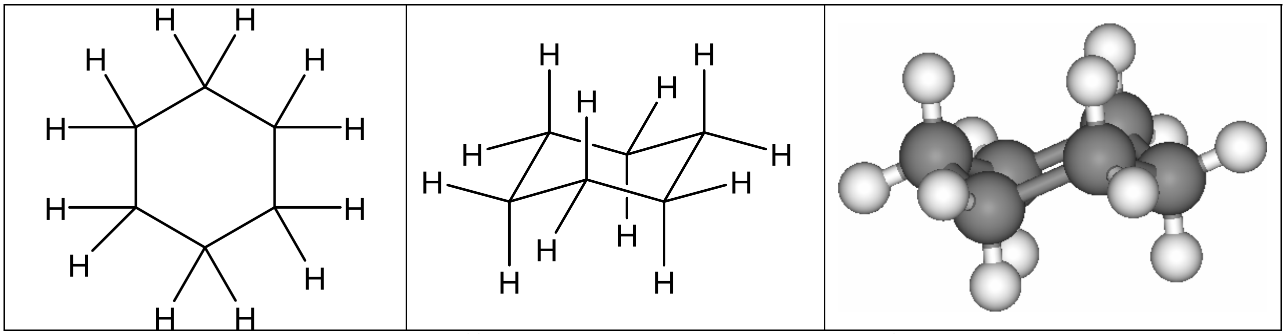


Figure 1. Three different pictorial representations of cyclohexane.

Students often have difficulty visualizing and interpreting these abstract symbolic representations because stimulation of meaningful thought processes usually is greatly dependent on sensory information (*2*). Students' struggles with visualization are especially pronounced when they are asked to move freely between two-dimensional and three-dimensional representations of molecular structure (*3*). Without strong conceptual foundations and visual-spatial ability, translating 2D to 3D or performing mental manipulations on three-dimensional molecules can be an extremely challenging task (*4*). Being able to visualize molecules is crucial to assimilate the concepts taught in a chemistry classroom that establish meaningful structure/function relationships (*5*). Advances in technology have now made a powerful education tool available, which moves far beyond the customary ways that chemistry (especially structural aspects) has been presented to students. It is now possible to equip large lecture halls with the capability of showing animated molecules and molecular reactions in 3D. This allows an expert, the lecturer, to guide the students in real-time as they explore and establish the relationship between the full three-dimensional structure, and the property of interest for any sized molecule, functional group, or orbital, rather than trying to accomplish the same end while working always or mostly with 2D representations.

There are many means of representing molecules that are useful in today's classroom. Typical two-dimensional conventions to help students visualize molecular structure include hand-drawn representations via the dash/wedge convention on the chalkboard or overhead transparencies, and 2D drawing programs such as Isis Draw or ChemDraw for use with overhead projectors or projection of slides (Figure 2). The challenge of 2D illustrations is that they are static, fragmentary snapshots of a chemistry that is dynamic (*6*). Figures presented in 2D inherently lack the capability of making a pronounced impact on the development of many students' proficiency in reaching meaningful conclusions about structure-function relationships (*7*).

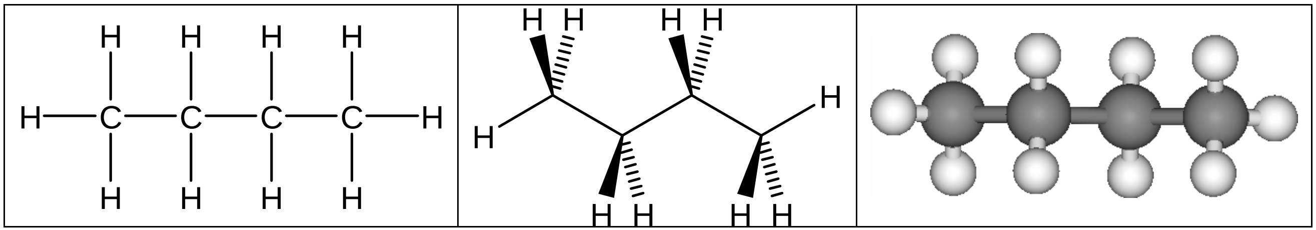


Figure 2. Three different pictorial representations of butane.

"Pseudo" 3D programs simulate 3D in two dimensions via strategic shading, careful perspective sizing, rotation, or a combination of these, to give 3D perspective. Programs, such as Chime, Rasmol, WebLab Viewer and all molecular modeling programs (e.g. PC Model, Chem 3D, MOE, Spartan, CAChe, etc.) undoubtedly help students in visualization, even though not "true" 3D (*8*). Figure 3 uses the browser plug-in Chime to display both cyclohexane in manipuable form, while Figure 4 uses the Jmol applet. Until now, the only "true" 3D teaching tools readily accessible to faculty in lecture halls have been physical models. While actual models more accurately convey structural information than 2D drawings, there is a practical limit to their use in lecture halls because they are large, hard to manipulate, and limited to smaller molecules (*9*). Additionally, physical models are not necessarily to scale, are challenging to animate, and cannot be changed between different representations (e.g., ball and stick, space-filling, etc.), so it is difficult to use them to portray the vibrant nature of molecules or the chemical processes they undergo. One advantage of physical models is that students can own a similar set, which provides a useful link between lecture and study.

Figure 3. Chime renditions of cyclohexane and butane.

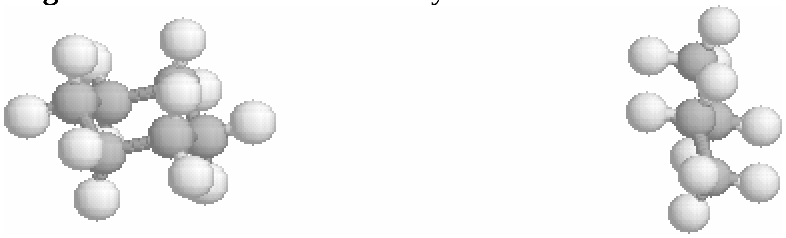
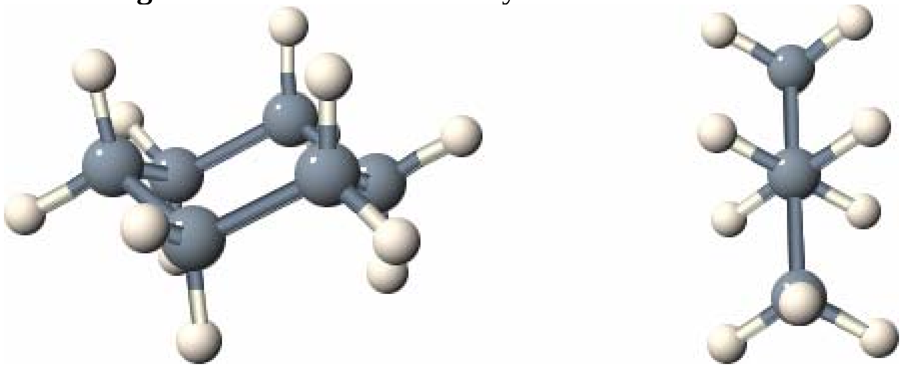


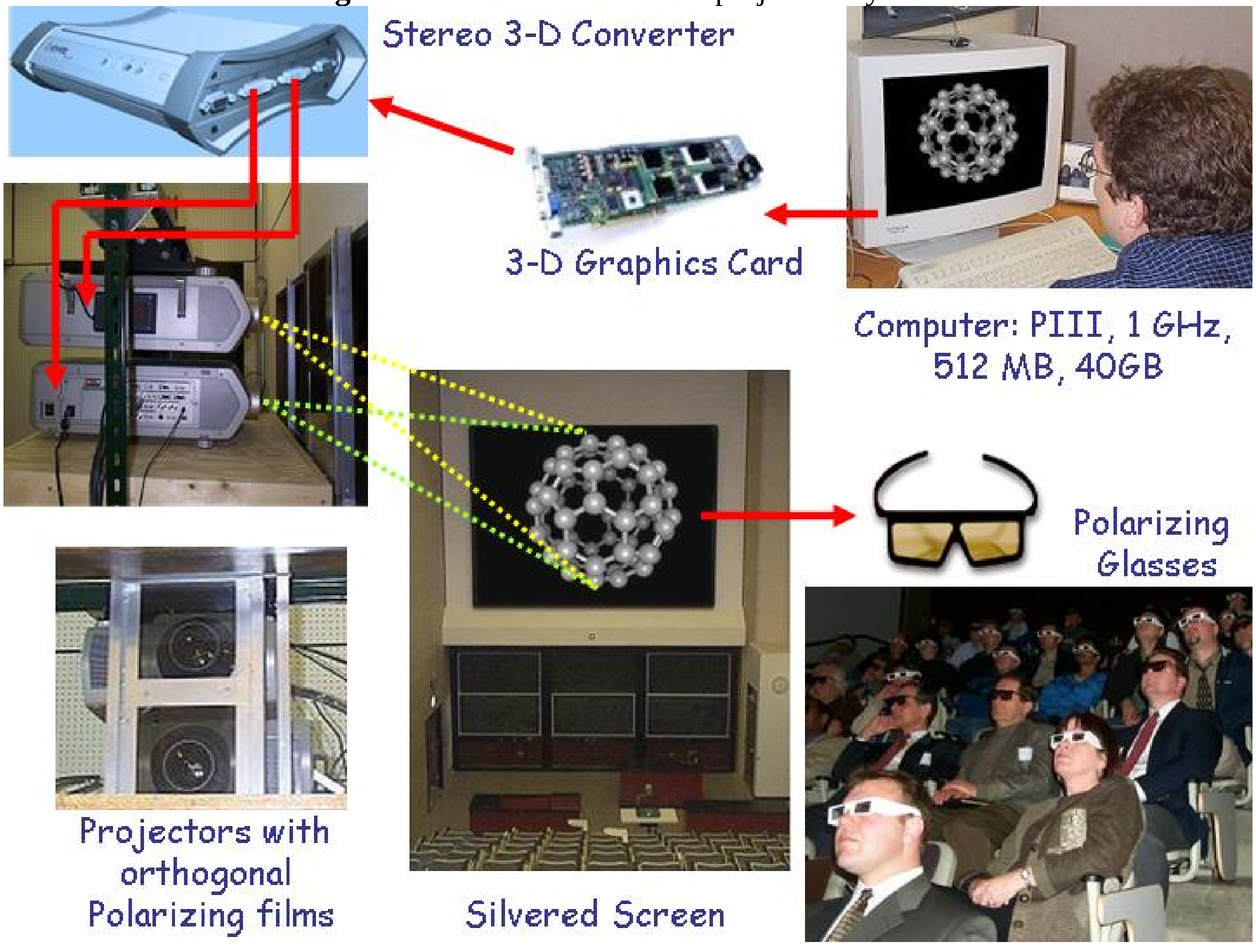
Figure 4. Jmol renditions of cyclohexane and butane.



Hardware – Overview, First Generation

It is now straight-forward and cost-effective to use modern technology to project computer generated three-dimensional images in large lecture halls using stereo projection. Figure 5 is a schematic of how the first-generation 3D system implemented in the Chemistry Department at the University of Pittsburgh worked. First, 3D models are computationally rendered using a software package such as MOE (*10*), or DS ViewerPro (*11*), among others. The 3D graphics card in the PC creates left-eye and right-eye images, in a frame sequential manner (sequentially and rapidly alternating between left eye and right eye images). That data stream is sent from the PC to a Cyviz converter (*12*) where the left eye image and right eye image (being generated by the PC) are separated and directed to two distinct, but overlapped and aligned projectors. Each image is then projected through a polarizing filter that is aligned at an orthogonal angle to its mate. This pair of polarized films matches the polarization of the glasses the audience is wearing, meaning that each eye is allowed to only see its corresponding image. When the two images are projected onto the silvered screen, the polarization of the images is retained when reflected back to the viewer, through their polarized glasses, and is seen. The brain then merges the right eye and left eye images into one image, and a 3D picture is finally “observed.” An auxiliary monitor at the lecturer’s bench receives a feed from one of the stereo outputs and allows the lecturer to see what is displayed (albeit in 2D) while facing the class.

Figure 5. Schematic of the 3D projection system.



Hardware – Details, First Generation

The lecture hall in which the 3D system is installed holds 125 students and is approximately 27’ (w) x 59’ (l) in size. Located in the front of the room is a lecturer’s bench that is fully equipped to meet the technological demands of modern lecture halls. Secured within the bench are the PC with LCD monitor, the Cyviz, and an electronics rack which houses the VCR, DVD, and cassette players (Figure 6). The computer is a 1GHz PIII with 512MB, 40 GB/7200 RPM hard drive, and floppy, zip, and DVD drives. We have found that the system works best when equipped with a large amount memory and the fastest processor possible. To display the 3D stereo images, a suitable graphics card is needed; the first generation system used the Wildcat II 5110 3D (see list on the Cyviz web site (*13*) for others that are compatible with that unit). The connection between the Cyviz and the video card involves a normal video cable and a special three-wire stereo control cable that carries the control signal specifying when the left-eye and right-eye images are coming through the video cable.

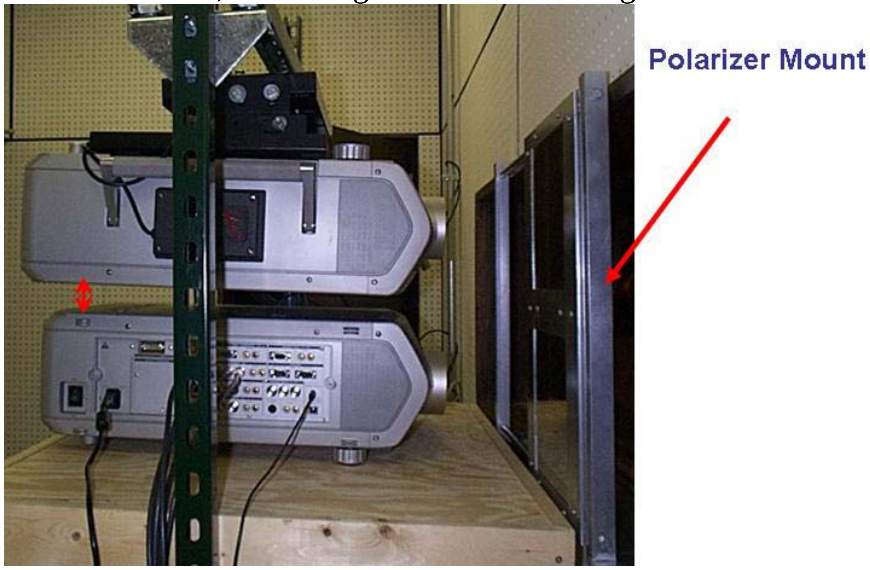
Figure 6. Photograph of the Lecturer's Bench with the "house PC".

The Cyviz Stereo 3D Converter is needed to separate and redirect the left eye and right eye images that the PC is generating. One issue faced was where to mount the Cyviz: next to the computer or 125' away from the computer and next to the projector (i.e., did one need one or two 125' VGA cables from the computer to the back of the lecture hall). It was decided to place the Cyviz converter near the "house PC". Fortunately, during a recent renovation to the lecture hall we had anticipated the eventual need for two projectors operating simultaneously from signal sources in the front of the lecture hall and thus the requisite wiring was already installed. The serial cable connection between the Cyviz and the house PC is available but it was found not to be necessary as the Cyviz operates perfectly without external control. (Since it was never tested, I remain unsure if I could have placed the Cyviz 125 ft (cable length) from the house PC without resorting to a signal amplifier for the stereo-control cable.)

We encountered several complications due to the Cyviz. The initial custom A/V wiring configuration of the lecture hall had all computer outputs from the lecturer's bench (house PC or lecturer's portable) sent through the Cyviz to the two projectors. When 3D is not being used, one of the projectors is turned off or blacked out, and the polarizers are removed from in front of the lenses. However, we have found that some laptop computers that work quite well with the projector directly, do not work when their external monitor signal is sent through the Cyviz (the problem is presumed to be due to incompatible refresh rates). This necessitated the rewiring of the lecturer's bench such that only the House PC output goes through the Cyviz and the portable PC output bypasses it.

The projection system that we use is composed of dual Sharp XG-v10XU Projectors with AN-LV55EZ Lenses (Figure 7). Each projector uses dual lamps with a combined brightness, per projector, of 4000 ANSI Lumens. Each polarizer allows 38% transmission of unpolarized light; thus the viewed image is noticeably less bright when a polarizer is in the light path. This necessitates either removing the polarizers when operating only one projector or using both projectors together even for non-3D uses. If one decides to use both projectors together, they must be in perfect alignment; otherwise the 2D image is too blurred to be of any use. We have found, however, that the alignment of the projectors does not have to be perfect for use in 3D mode, as the brain compensates for slight misalignments. If the projectors are not perfectly aligned, it is necessary to be able to use a single projector for non-3D applications without the polarizers. In the first-generation configuration, we manually had to remove/install the polarizers in the light path by slide the polarizer mount.

Figure 7. The dual projecting system: two Sharp XG-v10XU Projectors with AN-LV55EZ lenses. Note, the top projector hangs from the unistrut frame and the bottom projector sits on the table; this arrangement facilitates alignment.

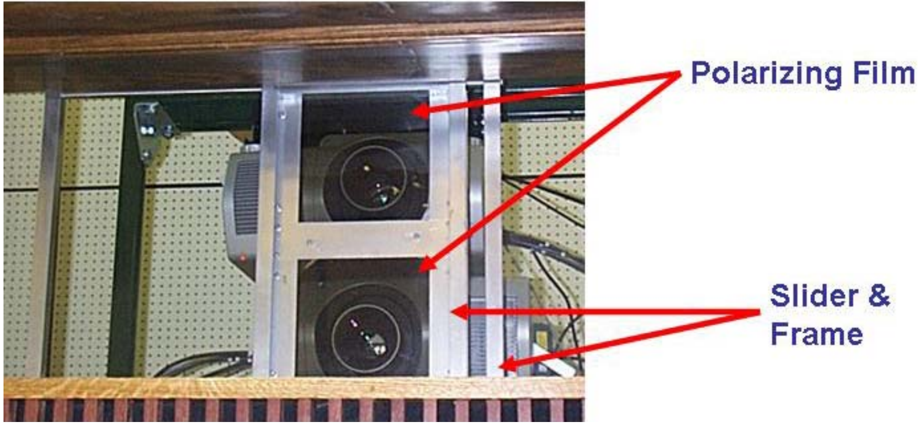


We had concerns about the aging of lamps: Should the lamps “age” at the same rate, and if one lamp is sufficiently brighter than the lamp in its mate projector, will that impact the 3D projection? Initially we thought that both projectors should be on even when only one was used (so that the bulbs should always have the same amount of usage). However, we have been running non-3D projection using a single (always the same) projector for many months, and have not noticed any degradation of the 3D image (i.e., differential bulb brightness does not seem to a concern).

Figure 8. The original polarizing films damaged by heat(1st generation polarizers).

The first set of polarizers that we used came with the Cyviz; our machinist fabricated simple aluminum frames to mount the polarizers directly onto the projector lenses (Figure 8; the polarizers were secured into the aluminum mounts by electrician's tape) due to polarizer size limitation. This method of mounting limited air circulation to one side of the polarizer only, which turned out to be insufficient to prevent heat damage to the polarizers. While replacement polarizing lenses could also be obtained from Cyviz, we chose to acquire the current set of polarizing films from Edmund Industrial Optics. Our machine shop next built the slider (Figure 9) to move the 9-inch square polarizers (larger size due to their location about 5 inches in front of the lenses) in and out of the light path; we have had no problems with this configuration. There are four different ways to install the "pair" of crossed polarizers. By trial and error we had to explore these before we had them matched to the glasses (i.e., you need the left eye data projector mated to the same polarizer as the left eye of the glasses). We have found that if the data projector polarizers are off by 45° from the glasses orientation (standard polarized glasses orient the film at 45° and 135°), dramatic color shifts become obvious and the 3D effect is poor. If the polarizers have the correct orientation, but are mismatched with respect to eyes, the images are obviously "confused" when viewed. We recommend checking the orientation before permanent modification of the polarizing film (we cut our first set with an incorrect orientation). If you are unsure if you are having problems with 3D, a simple check is to put the glasses on upside-down.

Figure 9. The linear polarizing laminated film on its slide mount (2nd generation polarizers).



A silvered screen is an absolute must for routine use, but aluminum foil will work for quick testing purposes. A standard projection screen does not work because it fails to retain the polarization of the reflected light. For the lecture hall, we purchased a Stewart Film screen (model # AT2M266CSLV3D) with "Silver 3D-(0")" screen material, an image size of 13-ft by 18-ft, an aspect ratio of 1.38:1, and a 14-ft by 19-ft frame (Figure 10). Installers must be warned not to touch the silvered surface, let anything else touch it, or if something comes in contact with the silvered surface, not to compound the problem by "wiping it off." It is prudent to use white gloves when handling the screen, and if you need to reinstall the screen, do not fold it, but cover the surface with clean paper and roll it around a tube.

Figure 10. The 13’x18’ silvered screen. Note the smudge due to installer’s error is visible at top, left-center of the screen.

The height above floor was of special concern to us. We were constrained by the lecture hall which dictated that the screen be wall-mounted 16’ above the floor (so all the chalkboards are always available (Figure 10), and 19’ from the first row, 36’ from the middle row, 54’ from the back row or chairs. It is awkward, with this configuration, for the lecturer to see the 3D image, but audiences from our demonstrations have concluded that the view from the front and back rows are good, with the middle rows being the best, presumably due to best vertical matching between the screen and the audience.

Initially, 130 pairs of polarized glasses were obtained from Vrex; 100 pairs of paper glasses ($0.69 each) and 30 pairs plastic glasses ($3.19 each). The paper glasses are too flimsy and too damaged for further use after 3-4 uses. One interesting point, however, was that the paper glasses are configured so that they worked regardless of how you folded them. While the plastic 3D glasses are more expensive, they are more durable and will save money in replacement costs in the long term.

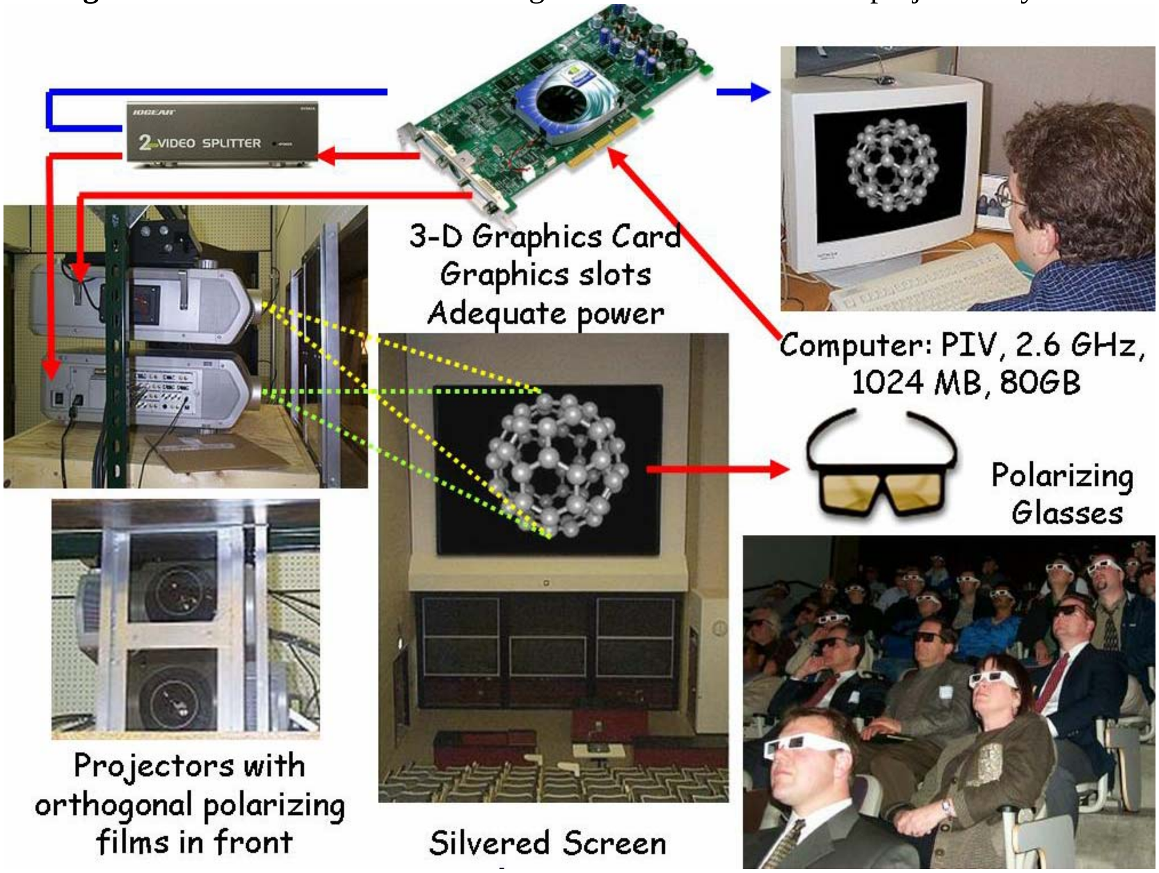
A green laser pointer was found to be a necessity because the traditional red laser pointers do not work well on silvered screens (which are too highly reflective). The green laser pointer still goes “through” the image, though. This means that the laser pointer is reflected on the sliver screen, but because the images are in 3D (and thus “come out at you”) the pointer appears to be going “through” the image. This makes it difficult to pinpoint certain features in a 3D image during discussions.

Links to many of the specific manufacturer's web sites for the items used to construct the system can be found on the our 3D Projection web site.

Hardware – Details, Second Generation

The second generation system used in the lecture hall is depicted in Figure 11. The significant changes are the replacement of the Cyviz unit with a dual-headed graphics card and powered video splitter (at a considerable cost savings), and the addition of a motor and associated circuitry to allow remote removal of the polarizers from the projected light path. The computer was also updated.

Figure 11. Schematic of the second generation lecture hall 3D projection system.



Software

The major software packages we use are Accelry's DS ViewerPro 5.0 (*14*), Chemical Computing Group's MOE (*15*), and Fujitsu's CAChe WorkSystem Pro 6.1.10(*16*). DS ViewerPro is the primary stereo viewer program used to date. Advantages to this program are that it can import many file types (i.e., pdb, mol, etc.) and convert them to 3D, it has animation capabilities, and it has an ActiveX component (which means it can be used to embed "pseudo" 3D structures in MS-PowerPoint). This package is also user friendly with a shallow learning curve which makes it attractive to lecturers. MOE also has stereo capabilities, as well as more sophisticated visualization capabilities, including the ability to show electron densities, molecular orbitals, charge density maps, and real-time minimizations in stereo mode. MOE can also import files generated by programs such as Gaussian or Spartan to project images derived from quantum mechanics. MOE's learning curve is more substantial than DS ViewerPro. The University of Pittsburgh recently purchased a site license for CAChe for a *Computing across the Chemistry Curriculum* project that spans all five campus locations. We have not yet, but will soon investigate using CAChe as our preferred stereo display software in order to minimize the number of different software packages a lecturer will need to know.

Modules

In appreciation of faculty time constraints an undergraduate started us on the process of creating 3D modules (see for example, Table 1) containing the images etc., to exploit the 3D system. It is our plan to use these modules to rapidly move beyond the "Golly Gee Whiz" aspect of the 3D system towards a more educationally effective pedagogy. Each module is designed as an add-in for standard lecture topics, and range in length from 3 to 10 minutes. Our ultimate goal is to enhance teaching effectiveness in every manner possible, so in addition, we are creating these modules with "real world" significance whenever possible. The modules are part of the tightly controlled "Molecules" web page we are building that is designed for Pitt faculty, according to the book used here and the examples they prefer to use in lecture.

Table 1. The initial set of educational modules designed.

Module Name	**Chapter**#	**Molecules included**
Thalidomide	Chapter 5	Thalidomide
Chirality	Chapter 5	Alcohols, (*R*)-Carvone, (*S*)-Carvone, (*R*)-Glyceraldehyde, (*S*)-Glyceraldehyde, and a stereogenic carbon
Benzene	Chapter 15	Frontier MO (6)
Ecstasy	Chapter 15	Ecstasy, Serotonin
Aromatic Molecules	Chapter 15	Benzene, Pyridine, Furan, Cyclooctatetraene, Planar Cyclooctatetraene, Buckyball, Hexahelicene

Vollhardt & Shore 3rd Edition.

Our Experiences

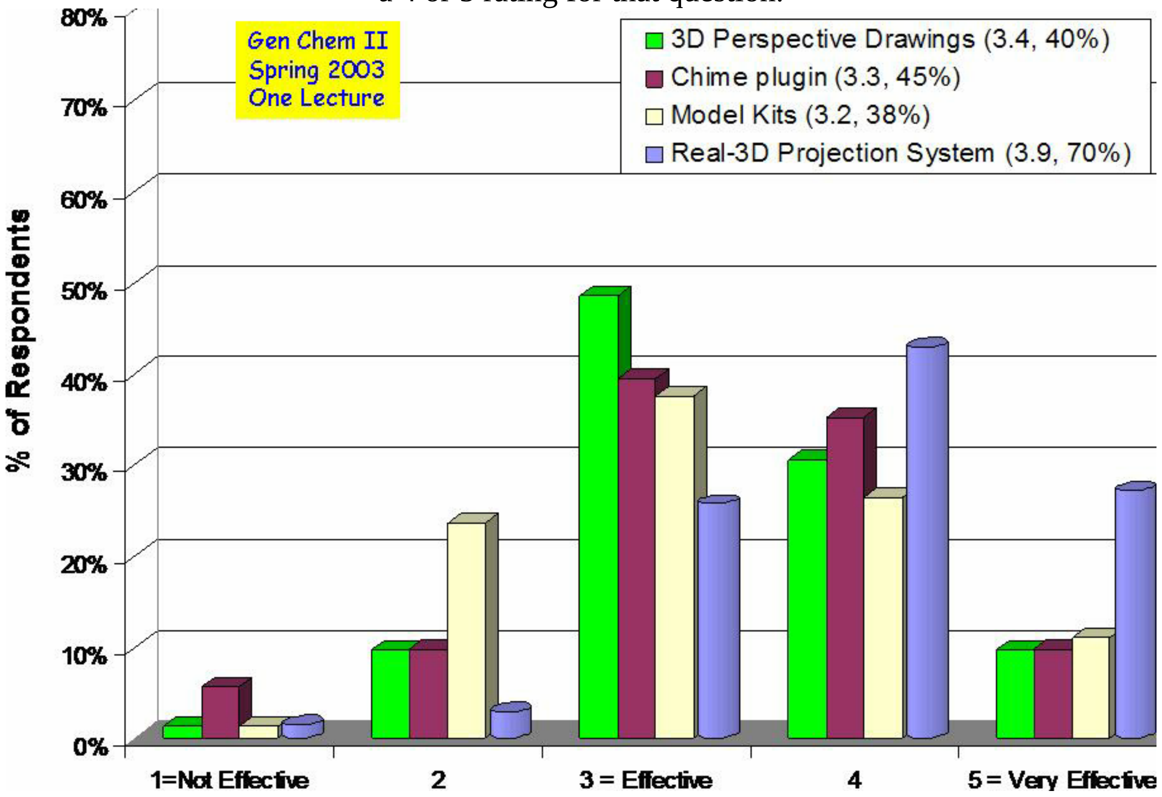
While this paper is designed to primarily discuss the hardware for performing 3D projection in the lecture hall, I did want to include a few comments about our experiences to date using the system. In addition to use in several Organic and General Chemistry courses, we have used the 3D system at functions such as the Chemistry Olympics, Alumni Events, and have received enthusiastic reviews. We understand that faculty time pressures are a limiting factor for new technology adoption, so we are creating modules to share. The educational value of the system is expected to be high, but one of our challenges will be to find a way to evaluate its impact on learning. If projecting 3D molecules and reactions only holds students attention a bit longer in lecture, the system has a value. Additionally, we believe in the statement that technology in the classroom empowers educators to reach a broader spectrum of students' learning styles (*17*). We hypothesize that it may enhance student understanding of the 3D reality of Chemistry, especially with repeated use. For the lecturer, using the 3D system is easier, faster, and more convenient than physical models. To enable faculty to easily present a module in the lecture hall, designed a Visual Basic program that launches 3D stereo molecules, organized by chapter title, at the touch of a button. This was initially envisioned as a crutch for self-announced technophobes. However, we have now abandoned that project and instead are focusing on a web page with materials stored in ".msv", which when clicked on, automatically launches the stereo display software.

While we have not yet secured the funding necessary to fully test the efficacy of 3D projection for teaching purposes have asked students in courses where the 3D system was used, to provide us some feedback. The small Organic chemistry class that I used the system in, and for which I requested unguided free response comments on the 3D system, generated these verbatim and representative comments:

- I greatly enjoyed the Real-3D because of the ability to have a greater understanding of how the molecules were rotated in space. The pseudo-3D was OK at this but not NEARLY as good.
- I might suggest more use of models in class. Seeing pictures is good, but so is hands on.
- It was really helpful when we discussed stereochemistry and substitution/elimination reactions. Seeing backside displacements and inversions in 3D really helped in the understanding in S_N2 reactions.
- Really helped me understand the class discussion of equatorial hydrogens in cyclohexane.
- Was so useful to me for understanding in the classroom, that it motivated me to use my model kit at home.
- All of chemistry is 3D so how can it not benefit me?
- Being able to see the bonds made and broken in the S_N2 animation helped me understand that mechanism much more than did the lecture models you used of the starting material, transition state, and product.

A General Chemistry II course, where the 3D system was used in one lecture, and in one recitation in the middle of the semester, an opinion survey administered on the final day of class generated the data shown in Figure 12 in response to the question (survey question #12) "*Rate the following four tools as to their effectiveness in helping you understand and visualize the three dimensional nature and interactions of molecules*". That students in that course also used the Chime plug-in to visualize structures (via the course web site), used 3D perspective drawings as is standard in general chemistry, and used models for one required laboratory. For whatever reason, the students clearly felt the expert-guided use of the 3D projection system in the one lecture and the one recitation was the most valuable tool, by far.

Figure 12. Student opinion survey results (see text). The numbers in parentheses following each of the four different “tools” are a “gpa-like score” calculated for tool’s response (using 1 for Not Effective and 5 for Very Effective), followed by the percent of all respondents who selected a 4 or 5 rating for that question.



Those same students responded to the question “*Do you think there was a distinct advantage to using the* <u>*real-3D*</u> *projection system compared to relying on traditional 2D representations? Why?*“ with 90% selecting yes. The free responses to the “why” provided a wide range of answers, of which 52% could be classified as belong to one of these three responses:

- Seeing it visually helps me
- you actually get to see the molecules
- spatial relationships were more clearly represented and easier to understand

<u>Concluding Remarks</u>

We are now able to show 3D images of any object or scientific image for which a stereo pair of photographs exists or can be created. We already have found great public interest in the 3D system and anticipate the 3D usage may expand rapidly since many lecture halls are already equipped with the first LCD projector and a computer. We have found it necessary and advantageous to extend the use of our 3D capabilities by designing a portable system (Figure 13) for use on the road and for faculty office practice (via shutter glasses). The portable system is basically the same as the permanent system, however on a smaller scale that is easily moved to any room within the building and which has been used at our local science museum and at the ACS meeting in Philadelphia in August, 2004. The first generation portable system was composed of a cart, shutter glasses capable of viewing images on the monitor in 3D, a fully equipped PC with graphics card, two mounted polarizing films, the Cyviz (a single unit is shared between the fixed and portable systems), two LCD projectors, and a portable Diplomat Projection Screen (Draper; this is an old screen we scrounged up) that extends approximately 70''x 60''. The second generation system utilizes a dual-head graphics card (Nvidia Quadro4 980XGL 128MB AGP Graphics Card) in place of the Cyviz unit. Details and links to all of the suppliers we used can be found at our web site at: http://chemed.chem.pitt.edu/3DProjection. Due to the decreasing absolute costs and the relative cost effectiveness of the system, we believe that 3D-equipped classrooms will become the new standard for teaching chemistry in today's universities.

Figure 13. Two different views of the portable cart housing the Cyviz, PC with graphics card,and mounted polarizing films (1st generation system), and the portable silvered screen.

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