Three-Dimensional Images in the Classroom

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Recently many devices for the three-dimensional visualization of molecules have become available to chemists. This article will review some new methods that can be used to generate stereoscopic images using molecular modeling programs available on microcomputers and will describe techniques that allow the 3-D perception of molecules in the classroom. Only inexpensive filters and glasses and other easily accessible equipment are needed. The methods described here should be of interest especially to organic chemists and biochemists for teaching and describing the results of their research.

Introduction to Stereoscopy

Several generations have been delighted by the three-dimensional photographs made popular by Stereopticon and Viewmaster stereoviewers. These devices allow the simultaneous viewing of two photographs that differ only in the position of the camera that recorded the images. This coordination allows the simulation of binocular vision so that depth perception can be obtained. The discovery of stereoscopy, the technique of producing images that can be perceived in three dimensions, was made over 150 years ago by the English physicist Charles Wheatstone, the inventor of the Wheatstone bridge (*1*). The methods of 3-D imaging recently have become more accessible to the chemist, because it has become easy to construct stereoscopic images of molecules with the assistance of the computer. These images are encountered in journals and textbooks with increasing frequency (*2*, *3*).

Microcomputer Modeling Software

An appreciation of the 3-D structure of molecules is essential to understanding the physical and chemical properties of compounds. Molecular models provide enormous insight into the spatial arrangement of atoms. When constructing models of moderately complex molecules there may be an insufficient number of component parts available, especially when working with expensive model kits. Another consideration is the time that it takes to build the models, especially if more than one type is desired, and the space required to store them. Chemistry modeling programs that have become available on personal computers have overcome some of these limitations.[1] Once a computer representation of a molecule has been constructed, it is possible to switch from a wire frame display to a ball-and-stick or space-filling representation with the touch of a finger. Furthermore, the information can be stored and retrieved rapidly at a later time. Structures can be obtained interactively either by using energy minimization routines built into the modeling programs, or from Chemical Abstracts Service. CAS now provides 3-D information that has been calculated for organic compounds. Three-dimensional coordinates can be downloaded from the REGISTRY file of CAS ONLINE and the stereoscopic representations of the molecules can be displayed using the Alchemy II[1] molecular modeling software. This service provides a method of rapidly obtaining approximate 3-D structural drawings for millions of compounds (*4*, *5*).

Three-Dimensional Images

Although for simple molecules, it is possible to get an idea of the spatial arrangement of the atoms by rotating the two-dimensional image of a structure on the computer monitor, the addition of a stereoscopic image affords an enormous advantage by providing the means to perceive the image in three dimensions. Unfortunately, relatively few people are able to convert stereoscopic images into 3-D pictures with the unaided eye.[2] This problem can be overcome by using a reflecting stereoscope.[3] This device uses two coupled periscopes to bring the appropriate image to the corresponding eye. The reflecting stereoscope allows the 3-D perception of molecules in full color and works on printed or projected images. It is especially effective to use the device looking directly at the computer monitor, because the 3-D nature of the molecule can be appreciated fully even as it is rotated about any axis by the computer program.

From an instructional point of view, using the reflecting stereoscope while looking directly at the monitor is effective for one person. For groups, the same method can be used by connecting the computer to a liquid crystal display device that allows the computer image to be projected as a transparency by an overhead projector. The audience directs the stereoviewer toward the projected image. The cost of the projection device and the many stereoscopes required is a serious disadvantage of this method. Alternative approaches that use inexpensive glasses are available for 3-D imaging for larger groups, and these will be described below.

3-D in the Classroom

In order for a larger audience to perceive 3-D images simultaneously, it is necessary to obtain a stereo pair of images of an object that can be projected with either overhead or slide projectors. Various methods have been proposed for obtaining the images (*9–20*). With the increasing availability of computers, it has become easy to obtain these by plotting the images onto a transparency using a computer plotter.[1,4] The overhead projection transparency can then

[1]For IBM compatible computers and the Apple Macintosh, *Alchemy II* is available from Tripos Associates, Inc., 6548 Clayton Road, St. Louis, MO 63117; *PCMODEL* (IBM and Macintosh II) is available from Serena Software, P.O. Box 3076, Bloomington, IN 47402-3076. For the Macintosh, *Chem3D* and *Chem3D Plus* are available from Cambridge Scientific Computing, Inc., 875 Massachusetts Ave., Suite 41, Cambridge, MA 02139. An inexpensive Macintosh program (*6*) *Molecular Editor* is available from Kinko's Academic Courseware Exchange, 255 West Stanley Ave., Ventura, CA 93001. *Alchemy II*, *Chem 3D*, and *Chem 3D Plus* can be purchased from the American Chemical Society, Distribution Office Dept. 56, P.O. Box 57136, West End Station, Washington, DC 20037.

[2]Some people can develop the skill of allowing each eye to see only the stereoscopic image that is directly in front of it. An alternative approach is to use a crossed-eye stereopsis, i.e., forming the 3-D image by crossing your eyes while looking at the stereo pairs. The latter method is easier to learn and can be effective even with large images; no viewing devices or special glasses are required (*7*). Stereo pairs that provide a correct image with a viewing device result in a mirror image perception when cross-eye stereopsis is used (*8*).

[3]Available from VCH Publishers, Suite 909, 220 East 23rd Street, New York, NY 10020-4606, and from Aldrich Chemical Company, P.O. Box 2060, Milwaukee, WI 53201.

be cut in order to separate the two stereo images. If two overhead projectors are available, no additional image preparation is necessary. One of the stereo images is placed on each overhead projector.[5] In order for each eye to see only the image intended for it, either complementary colored (red/blue or red/green) filters or polarizing filters must be placed in the light path. The two projected images are then superimposed on the projection screen. If a red filter is placed over one image, and a blue or green filter is placed over the other, 3-D image perception can be achieved with inexpensive glasses that have one red and one blue or green lens.[6] The left image and the left eye should both have the same color filter. The major limitation of this anaglyphic approach is that monochromatic images are obtained.

A similar approach can be used to obtain 3-D images in color. The same images that are used in the colored-filter method can be used, but different filters are used on the overhead projectors and in the glasses. Polarizing filters[7] transmit light of all colors, but if a perpendicular orientation of the filters is used for the left and right eyes, only the correct image will be seen by each eye. The orientation of the filters and glasses must be the same for each eye. This method requires the use of a reflective projection surface such a silver lenticular screen. It does not work with matte white or glass beaded projection screens since polarization of the light is lost on reflection from the surface.[8] With the correct projection screen it is possible to experience the full color of the 3-D images.[9]

The projection methods described use two overhead projectors and have the advantage that no special photographic equipment is required. A limitation, however, is the need to align the stereo pairs for each projected image. This method may be inconvenient when many molecules are to be shown. The alignment problem can be overcome using an infrared (Thermo-fax) transparency maker[4,10] to produce red and blue images on a transparent background, as described by Crozat and Watkins (*11*). An overlay of the two transparencies can then be shown on a single overhead projector, although color information is lost. This technique is effective only if special filters that match the red and blue colors of the transparency films are used in the glasses and if the image consists of line drawings (*11*).

Other ways to achieve alignment of the stereo pairs using slide transparencies have been described (*1, 2, 12, 13, 18, 20*).[11] As an alternative to photographing mechanical models, photographic images of the stereo pairs can be obtained directly from the computer monitor using a tripod-mounted camera in a darkened room. This approach is compatible with the use of polarizing filters and glasses and retains color in the images. If the availability of a lenticular projection screen is a concern, red and blue slide transparencies can be made using diazo dye film as described by Chang (*13*). These stereo pairs can be overlaid in a single mount, so that only one projector is required.

Conclusion

With the increase in availability of microcomputers and plotters, it has become easy to generate stereoscopic overhead or slide projection transparencies of molecules. The stereoscopic images can be perceived in 3-D by individuals with a reflecting stereoscope, or by students in a classroom using relatively inexpensive colored or polarizing filters and matching glasses to ensure that each eye sees only the correct image of the stereo pair. Techniques are described that do not require elaborate image preparation or equipment and provide an innovative way to present large 3-D models to a classroom.

[4] If a plotter is not available, the image can be printed using a color or black and white printer. Overhead projection transparencies can be made with inkjet, laser, or dot matrix printers by using computer graphics films that are available from 3M, 3M Austin Center, P.O. Box 2963, Austin TX 78769-2963. Alternatively, an infrared transparency maker (also available from 3M) can be used to produce a transparency from the printed image.

[5] Alternatively, two projection lenses can be attached to one overhead projector as described by Hayman (*14*).

[6] Red/blue or red/green glasses and filters can be obtained from Reel 3-D Enterprises, P.O. Box 2368, Culver City, CA 90231. Filters are also available from Edmund Scientific Co., 101 E. Gloucester Pike, Barrington, NJ 08007-1380. If cost is a consideration, red and green cellophane also can be adapted for this purpose.

[7] Inexpensive polarizing glasses can be obtained from Reel 3-D Enterprises. Polarizing filters can be obtained from Edmund Scientific Co. See footnote 6.

[8] Projection screens can be tested easily for the loss of polarization on reflection using a flashlight and two polarizing filters. Place one filter over the flashlight and the other between the reflected light and your eye. If light can be filtered out by rotating the second filter, that screen can be used with this method.

[9] Pointers cannot be used in the ordinary way with stereoscopic images. An effective use of a pointer for stereoscopic images has been described (*21*).

[10] Infrared transparency films that provide red, blue, or green images on a clear background are available from 3M. See footnote 4.

[11] A catalog of 3-D stereo slide formats, hand-held viewers for slides and prints, and other 3-D photographic accessories and supplies is available from Reel 3-D Enterprises. See footnote 6.

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