

Chem-Ray: A molecular graphics program featuring an umbra and penumbra shadowing routine

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Chem-Ray, new molecular graphics program, utilizes a combination of standard algorithms developed for molecular systems as well as various ray casting techniques to produce highly realistic images on inexpensive raster terminals. The program produces images of space-filling, ball and stick or stick models derived from a user-supplied coordinate list. The most notable new feature of Chem-Ray is a simple, yet effective, algorithm for the improved treatment of shadows within a molecule. This new algorithm is based upon a calculation of a light pyramid at each point under examination. Intersections of various objects with this light pyramid will decrease the percentage of the light that can reach the point. If the entire cross-section is blocked, the point will be in the umbra of the shadow; if only a portion of the light is blocked, the point will be in the penumbra of the shadow.

Keywords: molecular graphics, raster graphics, shadow algorithm

INTRODUCTION

The synthesis of a realistic image using computer graphics techniques is perhaps most dependent upon a proper treatment of the interactions of light with the subject. A proper accounting of shading, reflections and shadowing are necessary for an accurate representation. Sophisticated ray-tracing programs have evolved to the point where images can be produced in certain cases that are indistinguishable from actual images of the subject.¹ Unfortunately these methods are in general quite time consuming and are computationally expensive. Such methods are not readily applicable to interactive molecular modeling systems which require simple algorithms running at high speeds.

However, for close study, permanent record, and for publication, broadcast or seminar presentations, a highly realistic image is desirable and the amount of computing time required is not such an important question. A quality image allows the viewer to achieve a greater understanding of true three-dimensional structure of the molecular system under consideration. As the quality of the computed image improves with proper perspective, shading and shadowing, the need for a stereoscopic image decreases.

The computing equipment required for the production of a quality image has become readily available. Raster terminals or work stations of moderate resolution capable of displaying 256 colors simultaneously are sufficient and are now available for less than \$10,000. The computer requirements can be met by any available mini computer and by many enhanced micro computers.

In this paper I would like to describe Chem-Ray, a molecular graphics program that utilizes a combination of standard algorithms developed for molecular systems as well as various ray casting techniques to produce highly realistic images on inexpensive raster terminals. The program was written to be used in conjunction with existing interactive programs that allow on screen model building and structure manipulation. The most notable new feature in Chem-Ray is a simple, yet effective, algorithm for the improved treatment of shadows within a molecule.

The guiding philosophy behind Chem-Ray is the premise that chemistry is a structural science and that an accurate perception of structure will lead one to a better understanding of chemical properties and reactivity.

The subject

No one knows what a molecule looks like. This makes the creation of a realistic image of a molecule somewhat arbitrary. Chemists tend to think of molecules as represented by various physical models made of materials such as plastic, metal or wood. Traditionally molecular graphics programs create images of these models of molecules, with no attempt to create images of the actual molecules.²⁻⁴

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Three types of molecular models are commonly used by chemists: CPK space-filling models, ball and stick models and simple stick or Dreiding models. Each type of model has its own advantages. Space-filling molecules are good for evaluating steric interactions, but can make it difficult for an observer to quickly determine the chemical make up of the molecule. In a Dreiding model the chemical make up is obvious, but much spatial information is lost. Ball and stick models are very good for the construction of simple lattice structures, but are limited when it comes to molecules. Almost all commercial models are limited in the sense that only standard atom centers can be used; the models are built to represent average bond lengths and ideal angles.

A computer synthesized image of a model is not so restricted; actual bond distances and angles can be accurately modeled and the operator can easily switch from one kind of a model to another. Chem-Ray is written to produce images of the three main types of molecular models, based upon user-supplied coordinates.

The lighting model

The lighting model used in Chem-Ray is a modified version of the scheme discussed by Brickman.⁵ The light intensity of any point on a surface is the sum of diffuse and specular terms from each light source and an ambient term corresponding to nondirectional background light and to unaccounted-for light sources and reflections.

The diffuse light term, I_{diffuse} , is proportional to the cosine of the angle between the normal to the surface and the incoming light ray, I_{source} (see Figure 1 and Scheme 1). Light intensity falls in inverse proportion to the square of the distance traveled. In the program, the distance from each light source, d_{source} , is considered to be very large and the $1/d_{\text{source}}^2$ term is treated as a constant. The $1/d_{\text{view}}^2$ term is not constant and its effects provide valuable depth cueing. The R_{diffuse} term is the reflection coefficient.

The specular light intensity is a bit more complicated. If the surface was a perfect mirror, specular reflection would

$$I(i)_{\text{diffuse}} = I(i)_{\text{source}} * R_{\text{diffuse}} * 1/d_{\text{source}}^2 * 1/d_{\text{view}}^2 * \cos(\theta_i)$$

$$I(i)_{\text{specular}} = I(i)_{\text{source}} * R_{\text{specular}} * 1/d_{\text{source}}^2 * 1/d_{\text{view}}^2 * \cos^{2n}(\alpha_i)$$

$$I_{\text{observed}} = \sum_i I(i)_{\text{diffuse}} + I(i)_{\text{specular}}$$

be seen only at an angle, $-\theta$, corresponding to an incoming angle of θ . No surface is perfect and observed specular highlights are broader than mere points. A broadening term, $\cos^{2n}(\alpha)$, is used to give a smooth fall-off in specular intensity as one moves away from the ideal $-\theta$ angle.

The diffuse and specular terms from each light source are individually summed and multiplied by a shadow factor, $F(i)$, described in the next section. The intensity values from the diffuse and specular contributions from each light source are then summed and added to an ambient light term for an overall, $I_{\text{obs}}^{\text{total}}$, total intensity for the pixel that is output to the screen.

No mention has yet been made of color. The diffuse lighting terms are dependent upon the color of the object; the specular terms upon the color of each light source. The two sets of color must be combined for the final output. For the general case this requires a terminal capable of displaying a very large number of colors simultaneously. On a 256 color terminal this can not be done in the general case, too many different colors are needed. If the terminal is operated in a black and white mode, the color problem goes away and the 256 levels of gray are more than adequate for an excellent black and white image. But for a color image compromises must be made.

To avoid the color problem a simplified specular procedure is used with the calculated specular contribution replaced with an optional two color highlight. All pixels with $\alpha < \phi$ are given the color corresponding to the incoming light, most often pure white. Pixels with $\phi < \alpha < 2\phi$ are assigned the color with RGB values equal to the average of the RGB values of the incoming light and the brightest possible value of the diffuse light contribution at that point. The absence of the specular term is also compensated for by the use of a $\cos^2(\theta)$ term instead of the $\cos(\theta)$ term for the diffuse light contribution.

In the final implementation on a 256 color terminal two different lighting models are used. In the black and white mode, the unmodified procedures outlined in Scheme 1 are used, with different elements assigned different reflection coefficients. This mode is also used for generating halftone hard copy output. In the color mode, 30 color values assigned in the terminal color table for various shades of each atom color along with two values for the optional highlight. With 32 color table entries used for each atom color, a total

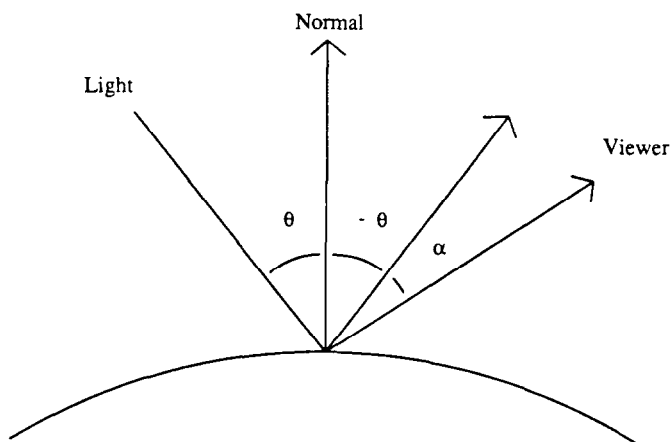


Figure 1. This drawing illustrates the angles used in Scheme 1. The incoming light ray makes an angle of θ with the normal to the surface. Perfect specular reflection would take place at an angle of $-\theta$; the viewer position is at an angle α from that position

of eight different atom colors can be used simultaneously on a 256 color machine. Using fewer than 30 color shades per atom introduces excessive color contouring.

Shadow routine

The inclusion of appropriate shadows within a picture is necessary for the production of a realistic image. If light sources are considered to be point sources then a shadowing routine is identical to the overlap routine used to determine the portions of the structure visible to the viewer. Only those objects "visible" from the light source will be lighted, all others will be in shadow. A separate calculation must be made for each light source.

Although simple to implement, point light sources are not very realistic. All natural light sources have width. The sun subtends an angle of about 0.5° in the sky. A typical room ceiling light fixture might subtend an angle of 10° . Light from a window will span an even greater angle. The shadows resulting from such light sources are softer than the hard shadows cast from a point light source. Shadows have both an umbra and a penumbra. An object is in the umbra of a shadow if the entire light source is obscured; it is in the penumbra if only a portion of the source is blocked. With a point light source there is no penumbra. As the width of the light source increases the umbra will decrease in size and the penumbra will increase.

A truly accurate modeling of shadow umbras and penumbras can be extremely difficult. The light distribution from a source in general is not uniform, many different objects may shadow the same point in space. Several different approaches have been used to determine shadows. One simple method is to use multiple point light sources to represent one source of finite width. This method is simple to use but the computational time goes up linearly with the number of point sources used. The method of shadow volumes has been used in which the intersections of various objects with the volume of space swept out by the possible light is examined.⁶ In a ray tracing program the light sources may be sampled by firing rays in random directions thus performing a Monte Carlo integration of the light intensity. Amanatides has developed a method that expands rays to the light source into cones.⁷ The intersections of various objects with the cones are used to determine the shadow umbra and penumbra. In Chem-Ray a simple variation of this latter technique is used.

To calculate the shadows using only a modest amount of computer time several approximations must be used. Considered in the abstract the various approximations seem rather drastic, but after implementation the overall effect is quite realistic.

Firstly, all light sources are considered to be square with a uniform light distribution, shining directly at the object being modeled from a relatively large distance away. Thus all light from a given source than can possibly strike a given point of the object will pass through the interior of a square pyramid, which has the square light source as the base and the point under consideration at the apex (see Figure 2). For the purpose of the calculations, the light source is considered to be at infinite distance; thus, the actual dimensions of the light pyramid are not specified. The angle subtended

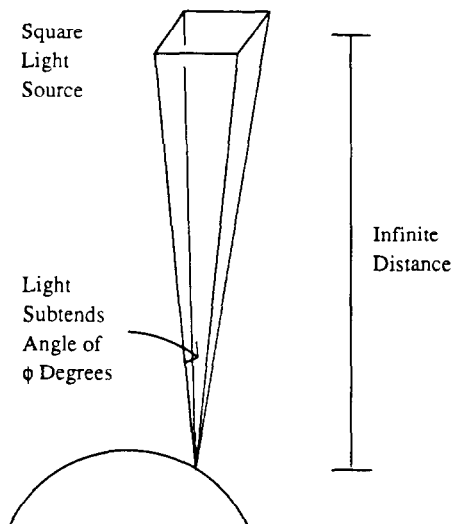


Figure 2. The light source is considered to be square with uniform light intensity at an infinite distance away. The light subtends an angle of ϕ degrees. The intersections of objects with this light pyramid will cast a shadow at the apex of the pyramid. If the entire cross-section of the pyramid is blocked then the point will be in the umbra of the shadow; if only a portion of the pyramid's cross-section is blocked then the point will be in the penumbra of the shadow.

by the light source is specified, thus fixing the dimension of any square cross-sectional slice of the pyramid.

Intersections of various objects with this pyramid will decrease the percentage of the light that can reach the point. If the entire cross-section is blocked, the point will be in the umbra of the shadow; if only a portion of the light is blocked, then the point will be in the penumbra.

Secondly, only the single intersection with the particular object that obscures the greatest cross-section of the light pyramid will be used to define the shadow factor $F(i)$. In the general case this approximation would not be a good one, but in practice in molecular graphics it causes only minor difficulties, since in most cases the sizes of the atoms and bonds are large with respect to the cross-sections of the light pyramid.

Third, the orientation of the light source is considered to float such that for any object penetrating the pyramid the front edge of the square cross-section will be parallel to the edge of the cross-section of the object. Since the atoms and bonds are large with respect to the cross-section of the light pyramid, the curvature of the edges of the bonds and atoms is ignored and the edges are considered to be straight lines.

With all of these approximations the shadow factor, $F(i)$, may be easily calculated (see Figure 3). The fraction of the cross-section obscured by each object intersecting the light pyramid is determined. The shadow factor is set equal to the largest single fraction.

The consideration of only the largest single fraction does cause error, but it is scarcely noticeable in the final image. When shadows of two objects cross the screen, pixels at the intersection points are somewhat brighter than they should be, but the smoothness of the penumbra shading tends to

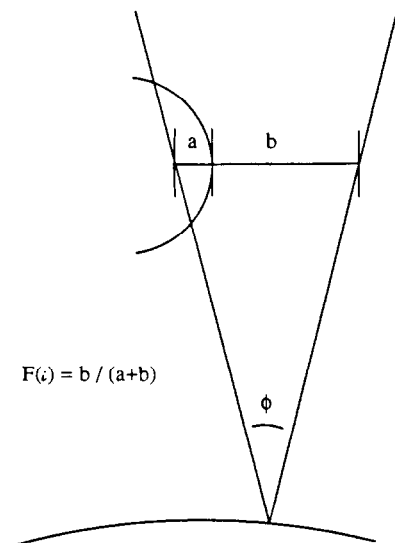


Figure 3. This drawing shows a cross-section of the light pyramid. If an atom or bond intersects the light pyramid, the shadow factor, $F(i)$, can be calculated using the relationship shown. If multiple objects intersect the light pyramid, only the single greatest $F(i)$ factor is used.

hide this fault. The floating orientation of the light source is not evident to the viewer and the assumption of an infinite distance to the light source is actually a good one since an actual molecular model held in one's hands would most often be lighted by distant light sources.

THE PROGRAM

The Chem-Ray program is written for raster terminals and produces an image by calculating color and intensity values for each pixel corresponding to each atom or bond in turn. A front to back algorithm is used, meaning that pixels belonging to atoms and bonds that are not visible are not calculated. Multiple light sources are allowed and the shadow umbra and penumbra are determined for each light source. A stepwise breakdown of the program follows:

- (1) The atom names and coordinates in orthogonal Ångström space are read in from a file, all atom selections, manipulations and transformations having been made previously in an interactive crystallographic or molecular modeling driving program. A bond connection table is read if bonds are to be drawn. The coordinates are scaled to pixel space and the atoms are assigned radii and colors based upon element type. The atoms and bonds are sorted, front to back;
- (2) A second set of perspective space coordinates based upon the viewer's position is determined. Bond and atom radii are also adjusted for perspective, with perspective causing the bond cylinders to be transformed to cones. A table of possible atom and bond overlaps is constructed;
- (3) A transformation of the original coordinates to a new coordinate system for each light source is made. Each light source is placed on the positive z axis of the transformed coordinate system at an infinite distance

from the molecule. In each of the transformed coordinate systems the atoms and bonds are sorted front to back and a new table of possible overlaps is constructed for shadow calculations;

- (4) The individual atoms and bonds are considered one by one, front to back. For each one the individual pixels covered by the atom or bond are examined individually. Each time a pixel is written to the screen, an entry in a logical array is made to prevent a subsequent write to that pixel. In many other programs pixels are considered scan line by scan line, but in Chem-Ray individual pixels are considered as they are encountered in the sorted atom and bond array;
- (5) The x and y coordinates of the pixel relative to the bond or atom center in perspective space are obtained directly from the screen, but the z coordinate must be calculated at each point. A check is made to see if the pixel is obscured by an atom or bond with a center at a lower z coordinate. (This is a common occurrence in the space-filling mode.) If the pixel is visible a transformation is made back to real space and then into the coordinate space of each light source;
- (6) Using the real space coordinates, the possible diffuse and specular light intensities contributed by each light source are determined using the equations of Scheme 1;
- (7) These possible intensities are then modified by the shadow routine that multiplies each possible intensity by a shadow factor corresponding to 1.0 for a pixel in the clear, to 0.0 for a pixel within the shadow umbra and to an intermediate value for pixels in the penumbra of the shadow;
- (8) The modified intensities are then summed and added to any possible ambient light contribution. A special simplifying treatment is given to the specular light, when the color capabilities of the terminal are limited;
- (9) The pixel is written to the screen and/or to a file and an entry is made in the logical array to prevent subsequent writes to the pixel;
- (10) The above steps are repeated for each pixel corresponding to the visible portions of each atom and bond in the molecule.

No pixel is considered more than once, pixels not covered by an atom or bond are never considered. The major storage requirements are sorted atom and bond lists for the main view and each light source and the logical array corresponding to the pixel dimensions.

The program speed is dependent upon the size of the image, the number of atoms and the number of light sources. An 800 by 800 pixel image of a DNA fragment of about 750 atoms with three light sources requires about 15 minutes of VAX 780 cpu time. Smaller molecules and calculations without the shadow algorithm are much faster. The program is not intended to be used for interactive graphics; very fast routines are available for that purpose.⁴

RESULTS

Chem-Ray is purely a graphics program. Thus it must be used in conjunction with other computer programs that allow on-screen selection and manipulation of atom coordinates.

At Stony Brook, Chem-Ray is used in conjunction with a number of different computer packages. These include modeling programs, such as Still's Macro-Model program⁸ or Chemical Design's CHEMGRAF package,⁹ and locally developed molecular mechanics programs designed for organometallics.¹⁰ Another important application is in conjunction with traditional crystallographic programs. Chem-Ray has been incorporated into Molecular Structure Corporation's TEXAN package.¹¹ In the TEXAN implementation, the molecule is oriented using an on-screen version of PLUTO¹² and the selected coordinates are written to a file for the Chem-Ray input.

The color plates show representative images from Chem-Ray. In each image an ambient light plus three distant light sources are used with a specular "white spot" corresponding to the brightest light. The orientations and relative intensities of the various light sources are varied from image to image.

Color Plate 1 shows a ball and stick representation of the molecule $[\text{Fe}_3(\text{CO})_{12}]$. The shadows are intentionally obvious in this picture in order to illustrate the effect. Normally, for a more pleasing image, a wider light source width and thus a more diffuse shadow would be specified along with a brighter ambient light.

Shadows can furnish important geometric clues to the viewer. Carbon monoxide will bond to the (110) face of a single crystal of nickel metal with a coverage of one CO per Ni atom. A space-filling representation of the geometry determined using molecular mechanics is shown in Color Plate 2.¹³ Notice how the shadows give depth and perspective to the CO ligands.

Chem-Ray is also useful for the presentation and analysis of unusual crystallographic results. Color Plate 3 shows a view of the cation, bis(cyclooctadiene) copper(I).¹⁴ The atoms are drawn at 80 percent of the accepted van der Waals radii. At 100 percent, the atoms of the two cyclooctadiene ligands almost completely obscure the copper atom. The cation is very crowded with longer than normal metal-carbon bond lengths.

To show the versatility of the program, Color Plates 4 and 5 illustrate two structures from the literature. Plate 4 shows a small section of a DNA strand. The C-G base pair at the top of the molecule can be clearly seen, with the shadows again providing important depth and perspective information. Finally, Plate 5 illustrates the lattice of the

high temperature superconductor, $\text{YBa}_2\text{Cu}_3\text{O}_7$.¹⁵ The defect perovskite lattice has a three layer structure with puckered outside layers of five coordinate Cu(II) cations, and an inner layer of four coordinate Cu(III) cations. The Ba(II) cations are between the inner and outer layers, while the Y(III) cations set between one three layer section and the next.

CONCLUSIONS

A molecular graphics program, Chem-Ray, has been written using a combination of traditional molecular graphics methods as well as various modern ray-tracing techniques. The program is capable of producing highly realistic images on color raster terminals. The most significant new feature of the program is a simple, yet effective, shadowing routine that simulates both the umbra and the penumbra of a shadow.

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