An interactive biomolecule graphics system

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This paper describes an interactive biological macromolecule graphic system on the VAX-11/750 + Model75 image-processing system. It can display the structure of types of macromolecules on the color monitor, and various user-defined options are available. The display model can be either a stick-and-ball model or a space-filling model. The user can easily display windows, rotate and shift interactively. For the space-filling model, a light source can be adjusted to produce a satisfactory three-dimensional effect. A fast algorithm for shading processing is proposed based on the use of spatial correlation information.

Keywords: molecular graphics, computer graphics, 3D display

Received 28 June 1987
Accepted 14 July 1987

This molecule graphic display system was designed to provide biologists with both an overview and a detailed view of biological macromolecule structures. It was also intended to aid the computer design of biological materials.[1]

Biological macromolecules are multipolymeres that consist of polymers, which are basic genes (such as RNA, DNA, etc.) linked to each other. Although the kinds of macromolecules are unlimited as far as their structure is concerned, the genes they contain are limited to several kinds. Therefore, to generate a three-dimensional (3D) display of molecules, we need atom-position data; knowledge of gene structures; and information about the particular molecule to be displayed, which is used to generate links between atoms.

In this molecule graphic display system, the knowledge of gene structures is manually summarized and categorized in a file. When the program is running, the file is opened, and the knowledge is read into central memory and used to guide atom linking. Knowledge of those genes and molecule-structure data, together with molecule features, specify the picture of molecule graphics. Features include chains in the molecule, the gene numbers of each chain (at both ends), the number and kind of irregular atoms linking at each end of the chains, and the number and position of disulphide bridges (if any exist). In our experiments, the molecule data file includes the position of each atom and the gene type to which it belongs. These data files are from a biological molecule database.

SYSTEM SCHEMA

The system schema is shown in Figure 1. It works in an interactive manner. When running the system, the user first specifies a molecule data file and reads in the molecule knowledge. The system then displays selections in a menu, and the user can select any desired function to execute. After the execution, the system goes back to display-selection mode (drive mode).

In the Display Subset Select function, the user can select any contiguous subset in a chain. Three different display methods are available in the Display Level Select function: Level 1 uses a point to represent every gene set; level 2 uses three atoms, which are located in the main strain, to represent every gene set; and level 3 displays all atoms. The user therefore can get an overview of a molecule's structure by selecting display level 1 and get a detailed view by selecting display level 3. In the Display Model Selection function, two kinds of display models are available: a stick-and-ball model and a space-filling model. The stick-and-ball model uses discs and lines to represent atoms and linking in order to visualize the interstructure of the molecule. The space-filling model uses a 3D ball to represent each atom. The radius of the ball is the radius of van der Waals force. For a better stereo effect, the shading and light-scattering effects are also considered. The light source and sphere reflectance can be adjusted to convey the 3D structure.

With the Shift and Rotate functions, the user can analyze the 3D structure from any direction and shift or rotate part or all of the molecule to find the best docking position. Atom substitution and manual editing are also possible in this mode. In the display mode,

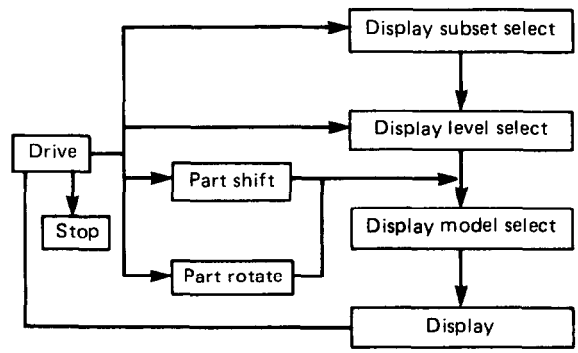

Figure 1. Block diagram of the display system

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can adjust the color of atoms and bonds and save the displayed image for later use.

HIDDEN-SURFACE ELIMINATION AND ILLUMINATION PROCESSING

Eliminating hidden surfaces is a primary problem of computer graphics. Here we use a raster-scanning algorithm. The basic idea is to separate the display plane into several parts, then eliminate hidden surfaces in each part.[2] More specifically, we divide the display plane into separate scanning lines and perform hidden-surface elimination on each scanning line. Each scanning line, in fact, is a projection of a plane with y-constant, known as the scanning plane, projected onto the plane z = zero (see Figure 2). The intersection of the scanning plane and the real object produces a set of intersection lines. To eliminate hidden surfaces, the user should process those lines and find out which parts of them are visible. The visible parts are then displayed, and the not-visible parts are eliminated.

In the case of the space-filling model, the intersection lines are in circular form, as shown in Figure 2(b). We define the point with its tangent parallel to the z axis and the intersection points as special points. Then the x coordinates of these special points partition the x axis into many unoverlapped intervals. Within each interval, one circle at most can be visible. For each interval, we take an arbitrary Xc within the interval and calculate the maximal of corresponding z of each arc using its

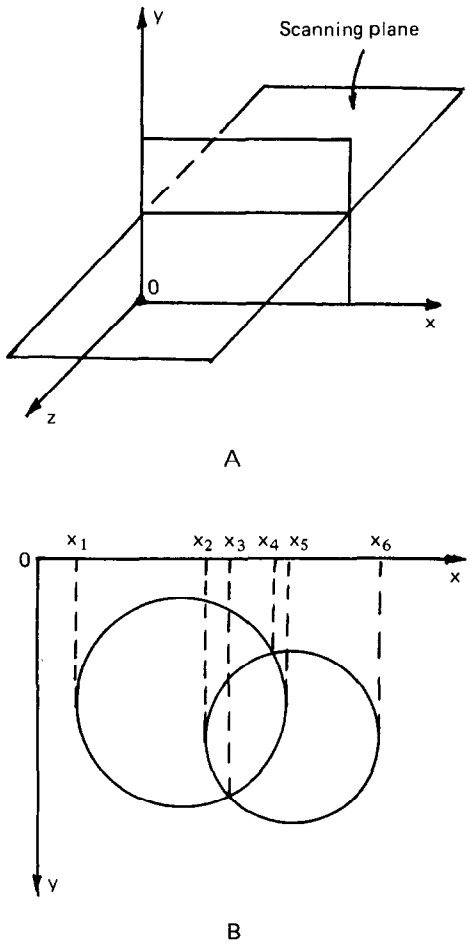


Figure 2. Scanning planes

Table 1. Visible codes

Interval	Code
0–X1	0
X1–X2	1
X2–X3	1
X3–X4	1
X4–X5	2
X5–X6	2
X6–	0

curve equation, then decide that the arc with maximal z value is a visible one. After processing all intervals, we get a list of interval visual codes (see Table 1). Visual codes 1 and 2 indicate that the corresponding circle numbers 1 and 2 are visible, while visual code 0 indicates that the interval is empty (there is no circle at all).

In fact, biological molecules usually contain many atoms. Therefore, many spheres may be overlayed in one perspective view. In this case, the hidden-surface elimination process may require too much time. To solve this problem, we propose a correlation algorithm that saves more than 60% of the computation usually involved.

The algorithm assigns a priority to each circle within the scanning plane. Visibility processes are then ordered according to their priorities. The visibility of each circle is first determined. If one circle is invisible, we proceed to the next one; otherwise, we find special points on the circle, partition the x coordinate into intervals, determine the visibility of each interval, and insert the visual code into a table according to its x coordinates. The priority assignment fully depends on the correlation of two adjacent lines. For each circle on the current line, we first check if it was visible on the last line. A highest priority is assigned if it was. Other priorities are assigned according to z coordinates. When determining the visibility of a circle, we first check if the circle is occluded by a circle already processed.

To gain stereo effect in the space-filling model display, the direction of light sources was designed to be adjustable. The gray level of every point of the sphere is calculated by a dense model. Here we employ Phone model[3], and the gray level is calculated by:

$$Sp = Cp[\cos(i)(1 - d) + d] + W(i)[\cos(s)]^{**}n$$

The first item represents the diffuse reflection and diffuse shine; the second item represents mirror reflection. Cp is a reflection coefficient, i is the input angle, d is the ratio of diffuse shine and diffuse reflection, s is the angle between input light and view direction, $W(i)$ is a weight factor (here we use the form of exponent), and n is a mirror reflection factor. The user can specify Cp, d, n, and light direction.

For simplicity, we assume that there is a light source at a point in infinite distance from the object and that the viewpoint is also far from the object.

EXPERIMENTAL RESULTS

Color Plate 1 shows three result graphs. A is a stick model of a DNA structure. B is a view of a nucleotide in DNA, which is selected and rotated to a user-defined angle by system modules. C shows a space-filling model of part of DNA. The system now is running on a VAX-11/750 + Model75 image-processing system.

REFERENCES

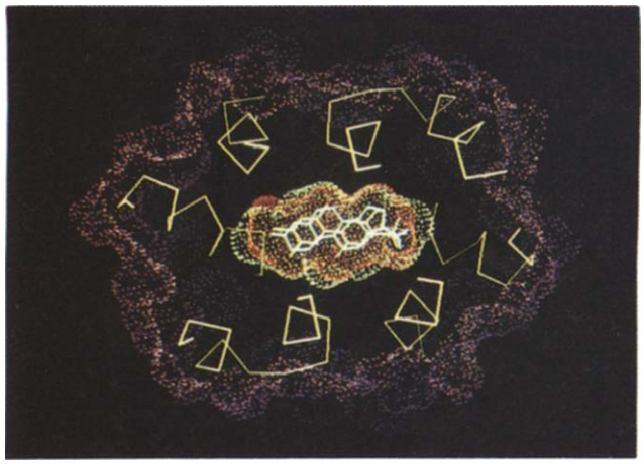
1 Molecular graphics abstracts, *J. Mol. Graphics*, 1984, **2**, 53–61

2 Mahl, Robert. Visible algorithms for quadric patches. *IEEE Trans. Computers*, 1972, **21, 1**

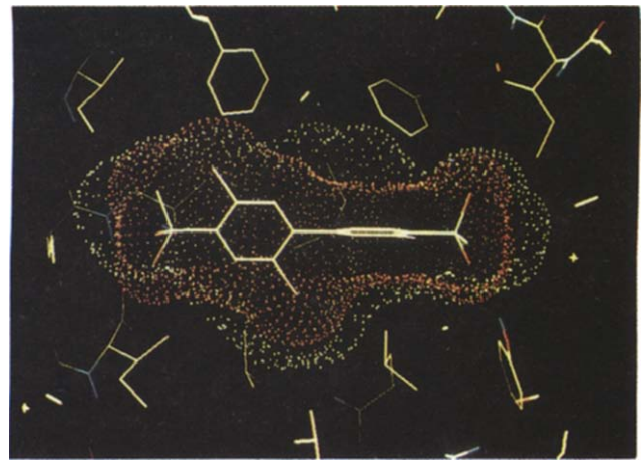
3 Phong, B. T. Illumination for computer generated pictures. *Communications of ACM*, 1975, **18, 6**

C. Cambillau and E. Horjales

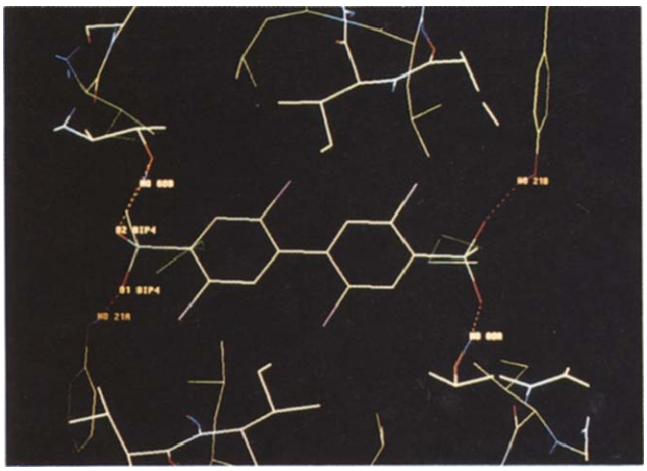
TOM: a FRODO subpackage for protein-ligand fitting with interactive energy minimization

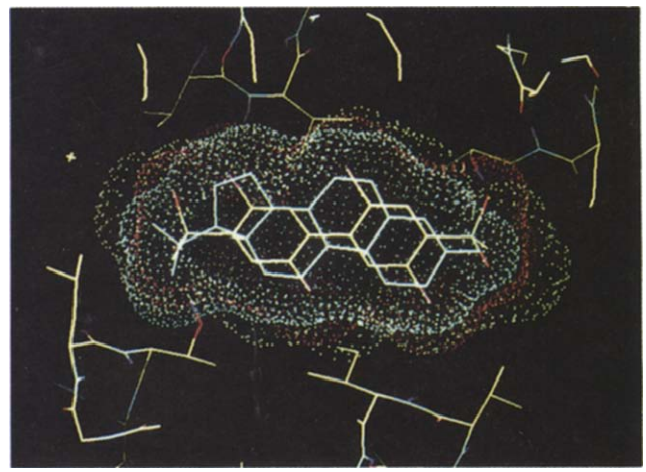


Color Plate 1. General view of the uteroglobin dimer, taken with its C2 axis perpendicular to the page. The yellow lines represent the alfa-carbon backbone. The water-accessible surface is displayed as violet dots (external surface) and green dots (internal cavity). The natural ligand, progesterone (in light blue) is superimposed after docking to the docked position of the inhibitor S²PCB (4, 4′-bis (methylsulfonyl)-2, 2′, 5, 5′-tetra-chlorobiphenyl) which surface is displayed in red



Color Plate 3. Comparison of water-accessible surfaces of progesteron (blue lines and dots) and S²PCB (red) after docking, with the one of the uteroglobin cavity (light green)

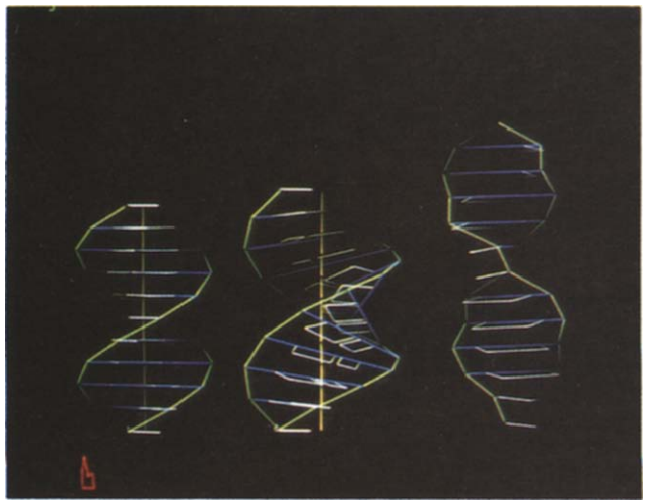




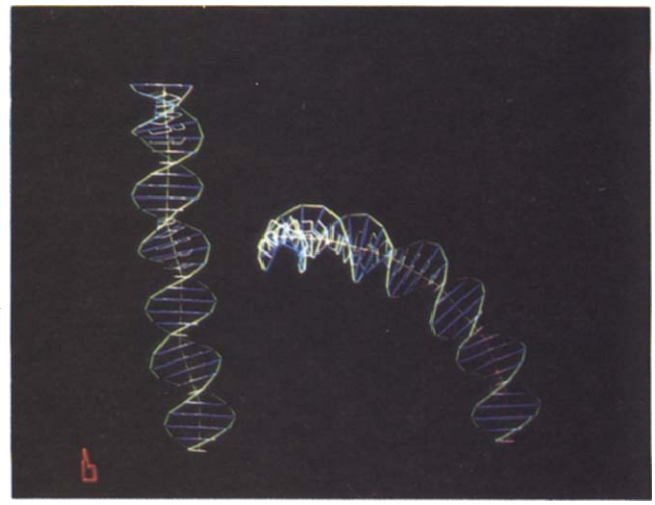
Color Plate 2. View of the S²PCB after docking in the uteroglobin cavity. (left) Very specific hydrogen bonds with tyrosines 60 and threonines 21 are displayed. The energy was found to be better than the ones for progesterone and other derivatives of PCBs. (right) Comparison between the water-accessible surfaces of the uteroglobin cavity (light green) and S²PCB (red)

Note: Color plates were taken on a Silicon Graphics IRIS 3020 workstation, using the FRODO version developed in the laboratory.

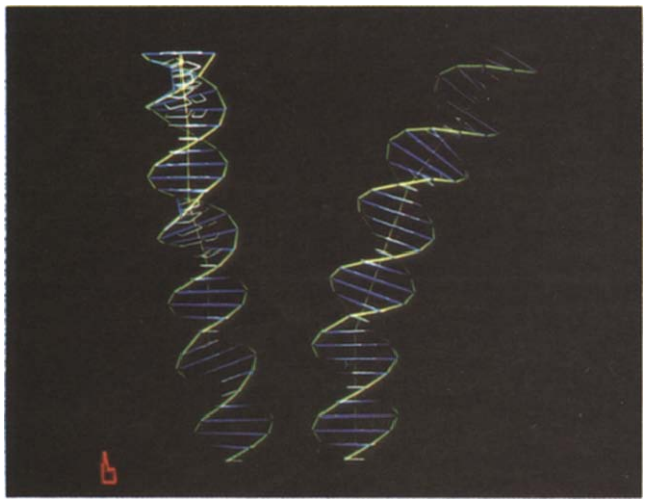
An interactive modeling program for DNA



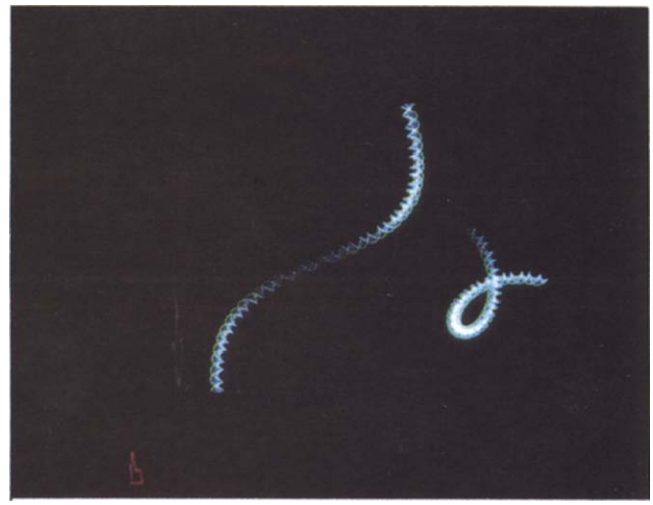
Color Plate 1. DNA in the standard forms A, B and Z from left to right. The twist angle is 36° in B-form and 33° in A-form; the roll angle is zero everywhere; the tilt angle is 0° in B-form and 13° in A-form; the propeller-twist angle is 0 everywhere



Color Plate 3. DNA in B-form in which the twist angle is 36° between all base pairs and the roll angle is 20° every n base pairs and zero elsewhere. From left to right: n = 5 and roll angle positive, the DNA is distorted but not bent; n = 5 and roll angle alternately positive and negative, the DNA is strongly bent



Color Plate 2. DNA in B-form in which the twist angle is 36° between all base pairs and the roll angle is +20° every n base pairs and zero elsewhere. From left to right: n = 5: the DNA is distorted but not bent; n = 10: the DNA is bent



Color Plate 4. DNA in B-form of sequence $(A_5T_5)_{20}$, in which the parameters are calculated on the basis of Tung and Harvey's model. The helical axis describes a left-handed superhelix

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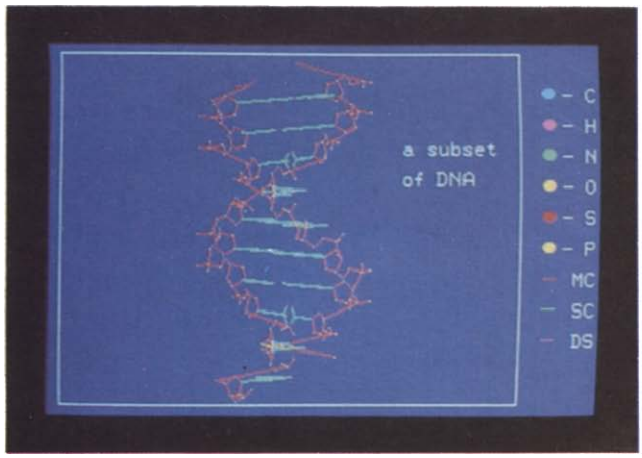

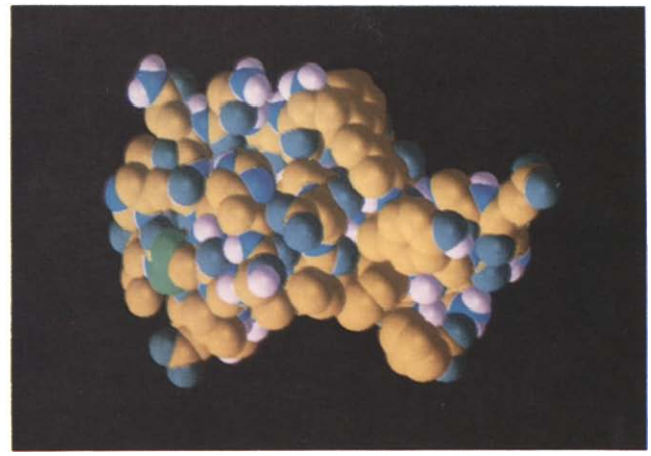

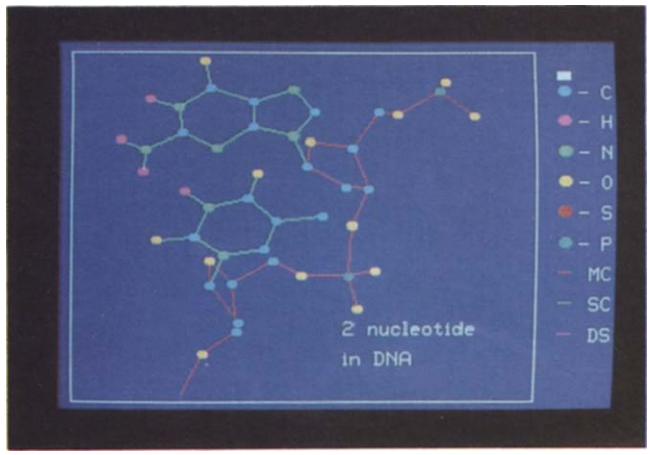

Color Plate 1. (above left) A stick model of a DNA structure; (left) a view of a nucleotide in DNA, selected and rotated to a user-defined angle; (above) a space-filled model of part of DNA

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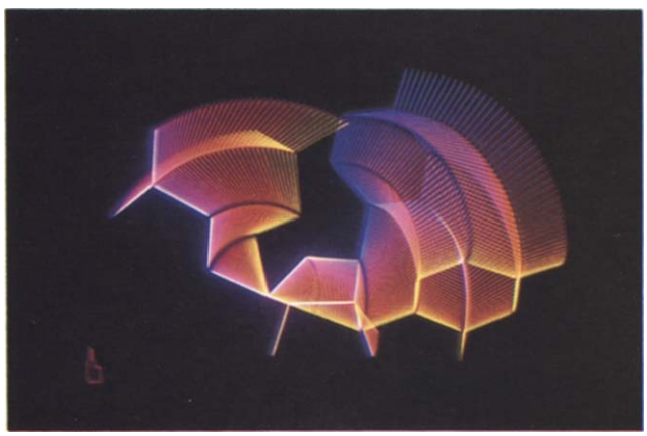
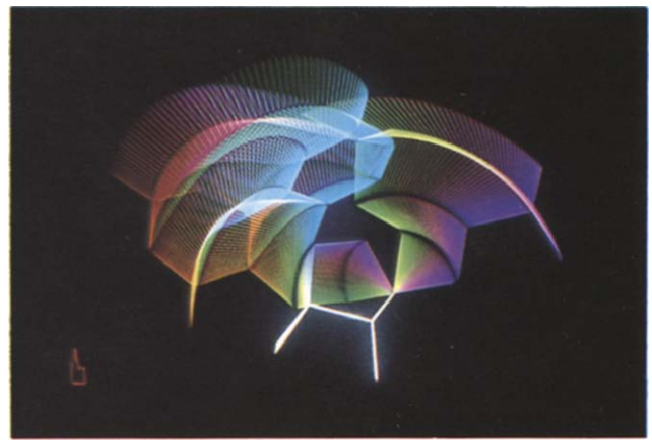


Color Plate 1. Pseudorotation from ideal conformation C2′-endo (in yellow) to ideal conformation C3′-endo (in blue). A step of 3° has been adopted while varying the phase of pseudorotation from 162° to 18°



Color Plate 2. Effect obtained when going through the complete pseudorotational pathway varying phase of pseudorotation from 0° to 357° with a 3° step

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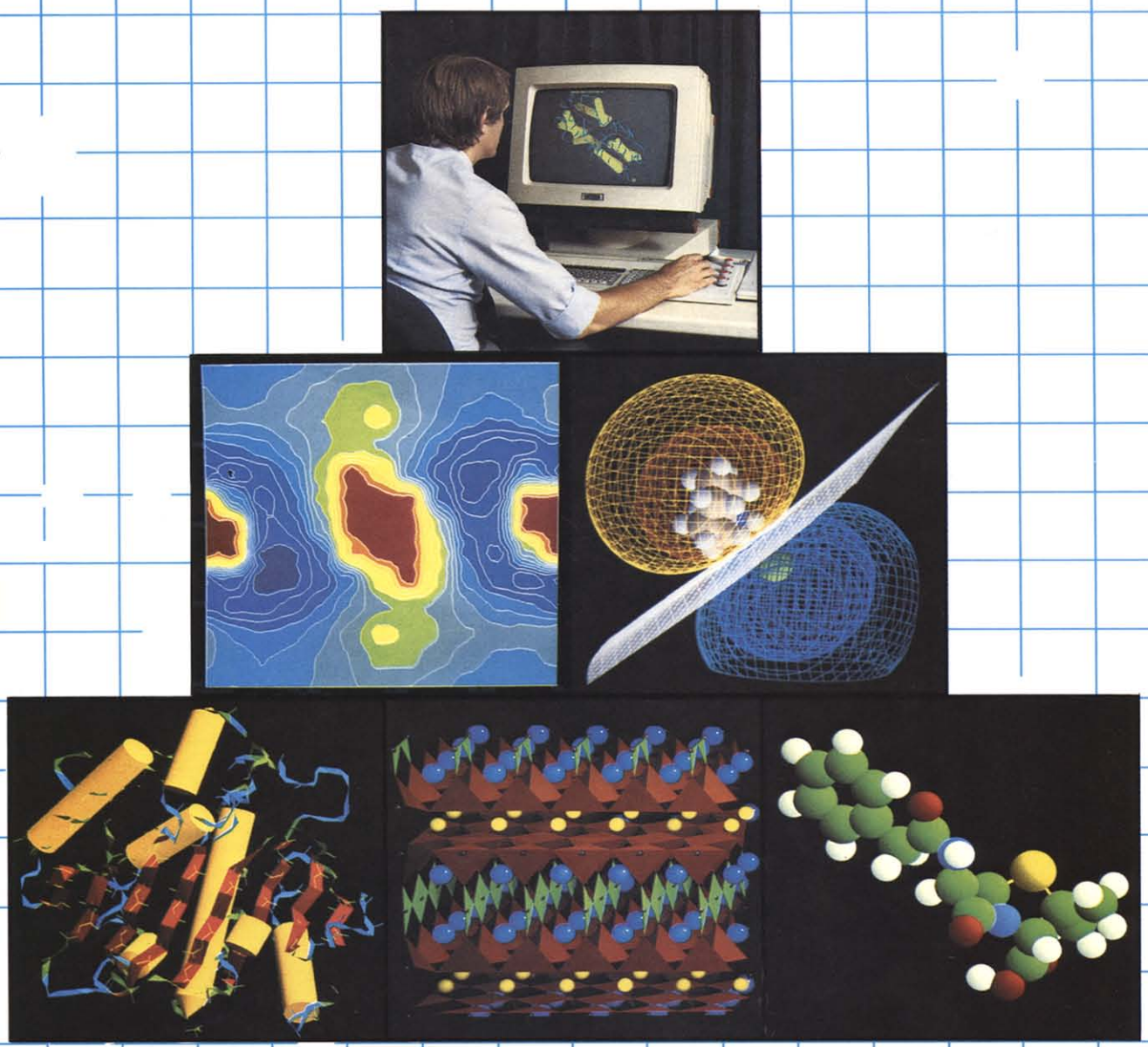

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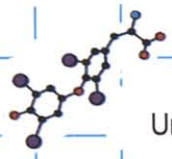

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