On the use of a general-purpose CAD program for molecular graphics

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It is suggested that general-purpose computer-aided design software can be of good use in producing high-quality molecular graphics. Such software is often widely available. Besides being an alternative to existing programs, hard copy creation is facilitated by this approach.

Keywords: computer graphics, software development, molecular graphics, computer-aided design (CAD)

INTRODUCTION

There is a great variety of computer programs for molecular modeling that allow on-screen display of different representations of molecules. Besides these general purpose programs specialized software in molecular graphics is well established. Widely used programs of this kind include Pluto,[1] Ortep[2] and Schakal.[3] Normally the creation of high-quality hard copies, especially in color, is done by taking photographs of high-resolution screens. This is a rather laborious task.

In this paper we describe a small piece of computer code that customizes standard computer-aided design (CAD) software and that can produce high-quality graphical representations of molecules, especially shaded ball-and-stick models. In certain situations this offers some advantages: Most importantly, CAD software typically can drive a very large variety of output devices. It takes care of low- and medium-level operations like handling graphic primitives and rendering. Further, it is very easy to perform interactive modifications like introducing text and overlaying several pictures. Often CAD programs are readily available so that no or little additional costs arise. Frequently the same software and user interface can run on a variety of machines, from AT-class personal computers to powerful workstations, so that machine dependence is overcome to some extent.

In this paper we describe a possible implementation of these ideas. First, an overview of commercial hardware and software is given. Then we discuss the inputs and steps necessary for the production of a picture, and procedures to enable the CAD software to display molecular models. Finally, we present two examples. The appendix gives some information that is too technical to be mentioned in the text.

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HARDWARE AND SOFTWARE BASE

A typical hardware configuration that works fine with the software discussed in this paper would consist of a 80386-based personal computer and a standard postscript laser printer. (We use a Hewlett Packard LaserjetII with QMS Jetscript card.) If color hard copies are desired, a Hewlett Packard PaintJet printer (this is a medium-resolution color ink-jet printer) can provide color printing in an inexpensive way. (As of this writing, the total cost of this equipment is about $7000.)

```
(defun SETMOL ()
 (setvar "surftab1" 32)
 (setvar "surftab2" 32)
)
(defun 3dist (P1 P2)
 (sqrt (+
    (* (- (car  P1) (car  P2) ) (- (car  P1) (car  P2) ) )
    (* (- (cadr  P1) (cadr  P2) ) (- (cadr  P1) (cadr  P2) ) )
    (* (- (caddr P1) (caddr P2) ) (- (caddr P1) (caddr P2) ) ) ) )
)
(defun scalat (P)
 (setq ATSCAL 1.0)
 (setq ATOFF '(10.0 7.0 0.0))
 (list (+ (* (car P) ATSCAL)  (car ATOFF)  )
     (+ (* (cadr P) ATSCAL)  (cadr ATOFF)  )
     (+ (* (caddr P) ATSCAL) (caddr ATOFF) ) )
)
(defun ATOM (CENT R COL)
 (command "color" COL)
 (setq CEN (scalat CENT))
 (setq P1 (list (- (car CEN) R) (cadr CEN) (caddr CEN)))
 (setq AX (list (car CEN) (+ (cadr CEN) R) (caddr CEN)))
 (command "CIRCLE" CEN R)
 (setq C1 (entlast))
 (command "LINE" AX CEN "")
 (setq L1 (entlast))
 (command "revsurf" P1 AX "" "")
 (entdel C1)
 (entdel L1)
)
(defun CYL (AT1 AT2 RA1 RA2 RCYL CYCOL)
 (command "color" CYCOL)
 (setq A1 (scalat AT1))
 (setq A2 (scalat AT2))
 (setvar "surftab1" 24)
 (setvar "surftab2" 24)
 (setq ZERO 0)
 (setq AA1 A1)
 (setq AA2 A2)
 (setq RRA1 (sqrt (- (* RA1 RA1) (* RCYL RCYL) ) ) )
 (setq RRA2 (sqrt (- (* RA2 RA2) (* RCYL RCYL) ) ) )
 (command "ucs" "za" A1 A2)
 (setq PRRA1 (list ZERO ZERO RRA1) )
 (command "circle" PRRA1 RCYL)
 (setq C1 (entlast))
 (setq V1 (- (3dist A1 A2) RRA1 RRA2) )
 (setq P1 (list RCYL ZERO RRA1  ) )
 (setq P2 (list RCYL ZERO (- RRA1 V1) ) )
 (setq P3 (list ZERO RCYL RRA1  ) )
 (command "line" P1 P2 "")
 (setq L1 (entlast))
 (command "tabsurf" P3 P2)
 (command "ucs" "world")
 (entdel C1)
 (entdel L1)
)
```

Figure 1. File containing the LISP functions defining atomic spheres and bond cylinders

On the software side, the two commercial programs[4] AutoCad V.10 and AutoShade 1.1 were used. AutoCad is by far the most widely used CAD package. It is a general purpose two- and three-dimensional design and drawing program. AutoShade renders the pictures created by AutoCad. AutoShade is a menu or script file-driven program that is easy to use due to the few parameters needed to determine lighting and viewpoint. It is not a ray-tracing program but it produces similar, highly realistic solid images in relatively short computing times.

It should be mentioned that most of the better CAD programs commercially available can be programmed in a way similar to AutoCad. Some of them can render the pictures without additional postprocessing software.

MOLECULAR GRAPHICS SOFTWARE

Our software supports the creation of calott and ball-and-stick models. It will be seen that modifications are easy. At the beginning, information about the molecule to be drawn has to be written to a file we call the "molecule definition file." For example, to create a ball-and-stick picture of a water molecule one could use the following 8 lines of input:

```
(SETQ O   '(0.0 0.0 0.0))                    ; Assign the symbols O, H1, and H2 to
(SETQ H1  '(-1.0 1.0 0.0))                   ;  the coordinates given as triplets
(SETQ H2  '(1.0 1.0 0.0))                    ;  of real numbers.
(ATOM O  "1.0" "GREEN")                      ; Draw the spheres representing the atoms
(ATOM H1 "0.5" "RED")                        ;  defined above with radii of 1.0 and 0.5
(ATOM H2 "0.5" "RED")                        ;  and colors green and red.
(CYL O H1 "1.0" "0.5" "0.3" "BLUE");Draw bond sticks between the spheres.
(CYL O H2 "1.0" "0.5" "0.3" "BLUE");  The blue bond sticks have a radius of 0.3.
```

More details of the syntax used in this file will be given later.

Obviously, a program that preprocesses any other format or helps to evaluate symmetry information and so forth could be used to create the special format used above. This task will not be discussed here. Except for large molecules, where an automatic check of interatomic distances is convenient to create the bond sticks, we normally find it easier to create a molecule definition file simply by editing an old one. The molecule definition file is actually a program in the language LISP which is (in form of the dialect called AutoLisp) the underlying programming language of AutoCad.

After starting AutoCad the file containing the functions for balls and sticks is loaded. In a sense this file (called the "function definitions file") is the molecule-drawing program itself. It is listed in Figure 1 and discussed in detail in the next section. The molecule definition file is then loaded and interpreted. At this point a wire-frame representation of the model can be viewed for correctness and additional changes can be introduced interactively. In principle however, AutoCad serves only to produce a file, which in its terminology is called a "filmroll file," that contains the information on the molecule to be rendered by AutoShade.

The user then starts AutoShade. After opening the filmroll file one typically interactively finds a suitable viewpoint (called the "camera position" in AutoShade terminology) and suitable lighting conditions (often the default values will be suitable), and creates a hard copy or a postscript file to be sent to a hard-copy device later.

FUNCTION DEFINITIONS FILE

The function definitions file shown in Figure 1 will be discussed in some detail because most readers are probably not familiar with LISP. This file is just a collection of some LISP functions, the most important being ATOM and CYL, which have already appeared in the previous section. For a comprehensive introduction to LISP the reader is referred to the section "AutoLisp programmer's reference" in the AutoCad reference manual.

The two variables *surftab1* and *surftab2* (lines 2 and 3) determine how many segments are used in the piecewise construction of spheres and cylinders. For the figures in this paper this value was always 32. The auxiliary function 3DIST (line 3) just calculates the distance between two points. (The standard AutoCad distance function calculates only the two-dimensional distance.) The function SCALAT (line 11) is used to uniformly scale and shift all atoms. The user might want to change the scaling factor and offset value, for example according to the length units used. The function ATOM (line 18) draws the spheres. This is done by rotating a circle around an axis, which is one of several ways of creating a sphere in AutoCad. Most of the work is done by the internal command REVSURF (line 27). ATOM requires as parameters the atomic position, radius and color of the sphere. The function CYL (line 31) draws the bond sticks. Due to an internal error in AutoShade one cannot let the cylinders start and end at the centers of the atoms and let the face-hiding algorithm remove those parts that are hidden inside the spheres. Therefore the cylinders are constructed first by calculating the intrusion points of the two spheres they connect and then giving them a three-dimensional thickness. CYL requires as parameters the positions and radii of the two atoms to be connected, the thickness of the bond cylinder and its color. After getting used to the syntax, the reader may find that this short procedure file is easily modified and adapted to special needs.

EXAMPLES

Two examples shall illustrate the molecule definition file and show the corresponding output. Figure 2 contains the

```
1  (defun IW8 ()
2  (setmol)
3  (setq O1 '(  0.0000  4.0087  4.0087 ))
4  (setq O2 '( -4.0087  0.0000  4.0087 ))
5  (setq O3 '(  0.0000 -4.0087  4.0087 ))
6  (setq O4 '(  4.0087  0.0000 -4.0087 ))
7  (setq O5 '(  0.0000  4.0087 -4.0087 ))
8  (setq O6 '( -4.0087  0.0000 -4.0087 ))
9  (setq O7 '(  0.0000 -4.0087 -4.0087 ))
10 (setq O8 '(  4.0087  0.0000  4.0087 ))
11 (setq HO1 '(  0.0000  5.8027  3.7804 ))
12 (setq HO2 '( -5.8027  0.0000  3.7804 ))
13 (setq HO3 '(  0.0000 -5.8027  3.7804 ))
14 (setq HO4 '(  5.8027  0.0000 -3.7804 ))
15 (setq HO5 '(  0.0000  5.8027 -3.7804 ))
16 (setq HO6 '( -5.8027  0.0000 -3.7804 ))
17 (setq HO7 '(  0.0000 -5.8027 -3.7804 ))
18 (setq HO8 '(  5.8027  0.0000  3.7804 ))
19 (setq HE1 '(  0.0000  3.7804  5.8027 ))
19 (setq HE2 '( -3.7808  0.0000  5.8027 ))
20 (setq HE3 '(  0.0000 -3.7804  5.8027 ))
21 (setq HE4 '(  3.7804  0.0000 -5.8027 ))
22 (setq HE5 '(  0.0000  3.7804 -5.8027 ))
23 (setq HE6 '( -3.7804  0.0000 -5.8027 ))
24 (setq HE7 '(  0.0000 -3.7804 -5.8027 ))
25 (setq HE8 '(  3.7804  0.0000  5.8027 ))
26 (setq ION '(  0.0 0.0 0.0 ))
27
28 (setq ROHCYL 0.20)
29 (setq ROOCYL 0.15)
30 (setq RO 1)
31 (setq RI 1.5)
32 (setq RH 0.6)
33
34 (setq CYLOHC "YELLOW")
35 (setq CYLOOC "MAGENTA")
36 (setq OCOL "RED")
37 (setq HCOL "51")
38 (setq ICOL "CYAN")
39
40 (atom O1 RO OCOL )
41 (atom O2 RO OCOL )
42 (atom O3 RO OCOL )
43 (atom O4 RO OCOL )
44 (atom O5 RO OCOL )
45 (atom O6 RO OCOL )
46 (atom O7 RO OCOL )
47 (atom O8 RO OCOL )
48 (atom HE1 RH HCOL )
49 (atom HE2 RH HCOL )
50 (atom HE3 RH HCOL )
51 (atom HE4 RH HCOL )
52 (atom HE5 RH HCOL )
53 (atom HE6 RH HCOL )
54 (atom HE7 RH HCOL )
55 (atom HE8 RH HCOL )
56 (atom HO1 RH HCOL )
57 (atom HO2 RH HCOL )
58 (atom HO3 RH HCOL )
59 (atom HO4 RH HCOL )
60 (atom HO5 RH HCOL )
61 (atom HO6 RH HCOL )
62 (atom HO7 RH HCOL )
63 (atom HO8 RH HCOL )
64 (atom ION RI ICOL )
65
66 (cyl O1 HE1 RO RH ROHCYL CYLOHC)
67 (cyl O1 HO1  RO RH ROHCYL CYLOHC)
68 (cyl O2 HE2 RO RH ROHCYL CYLOHC)
69 (cyl O2 HO2  RO RH ROHCYL CYLOHC)
70 (cyl O3 HE3 RO RH ROHCYL CYLOHC)
71 (cyl O3 HO3  RO RH ROHCYL CYLOHC)
72 (cyl O4 HE4 RO RH ROHCYL CYLOHC)
73 (cyl O4 HO4  RO RH ROHCYL CYLOHC)
74 (cyl O5 HE5 RO RH ROHCYL CYLOHC)
75 (cyl O5 HO5  RO RH ROHCYL CYLOHC)
76 (cyl O6 HE6 RO RH ROHCYL CYLOHC)
77 (cyl O6 HO6  RO RH ROHCYL CYLOHC)
78 (cyl O7 HE7 RO RH ROHCYL CYLOHC)
79 (cyl O7 HO7  RO RH ROHCYL CYLOHC)
80 (cyl O8 HE8 RO RH ROHCYL CYLOHC)
81 (cyl O8 HO8  RO RH ROHCYL CYLOHC)
82
83 (cyl O1 O5 RO RO ROOCYL CYLOOC)
84 (cyl O2 O6 RO RO ROOCYL CYLOOC)
85 (cyl O3 O7 RO RO ROOCYL CYLOOC)
86 (cyl O8 O4 RO RO ROOCYL CYLOOC)
87 (cyl O1 O2 RO RO ROOCYL CYLOOC)
88 (cyl O2 O3 RO RO ROOCYL CYLOOC)
89 (cyl O3 O8 RO RO ROOCYL CYLOOC)
90 (cyl O8 O1 RO RO ROOCYL CYLOOC)
91 (cyl O4 O5 RO RO ROOCYL CYLOOC)
92 (cyl O5 O6 RO RO ROOCYL CYLOOC)
93 (cyl O6 O7 RO RO ROOCYL CYLOOC)
94 (cyl O7 O4 RO RO ROOCYL CYLOOC)
95
96 (command "redraw")
97 )
```

Figure 2. Molecule definition file for the cubically hydrated cation displayed in Figures 3 and 4

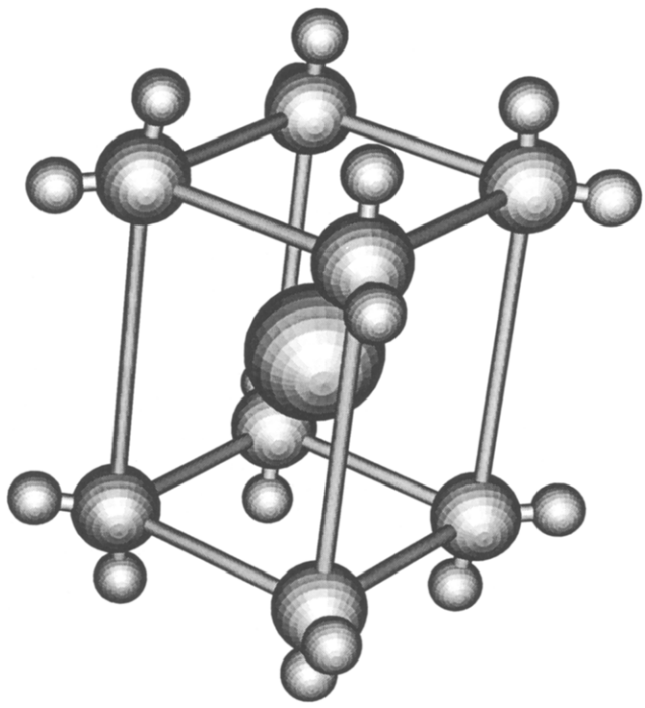

Figure 3. Output created on a postscript laser printer with 300-dots/inch resolution when the data of Figure 2 is processed by AutoCad and AutoShade

definitions for a picture of a cubically hydrated cation as plotted in Color Plate 1 and Figure 3. At the beginning, the coordinates of the atoms are defined (lines 3 to 26). The 5 commands starting from line 28 define the radii of the spheres for O,H, the central ion, and the thickness of the bond sticks. Then colors are defined for all of these entities. In AutoCad, colors can be assigned by names or numbers. The actual drawing of the atoms starts with line 40. From line 65 to line 90 the drawing of the cylinders is performed. The REDRAW command at the very end removes some spurious construction lines. AutoCad and AutoShade, respectively, without further modifications produced Color Plate 1 (color printer output with PaintJet) and Figure 3 (laser printer output).

The second example illustrates the possibility of modifying a molecular picture by superimposing a second one. A Pt_{13} cluster represents a fragment of a metal surface. The molecule definition file of this cluster is listed in Figure 4. It can be seen that nothing principal is different from the

```
1  (defun PT13 ()
2  (setmol)
3  (setq PT1 '(10.00  5.00 0.00))
4  (setq PT2 '(10.00 10.00 0.00))
5  (setq PT3 '(10.00 15.00 0.00))
6  (setq PT4 '(15.00  5.00 0.00))
7  (setq PT5 '(15.00 10.00 0.00))
8  (setq PT6 '(15.00 15.00 0.00))
9  (setq PT7 '(20.00  5.00 0.00))
10 (setq PT8 '(20.00 10.00 0.00))
11 (setq PT9 '(20.00 15.00 0.00))
12 (setq PT10 '(12.50  7.50 -4.00))
13 (setq PT11 '(12.50 12.50 -4.00))
14 (setq PT12 '(17.50  7.50 -4.00))
15 (setq PT13 '(17.50 12.50 -4.00))
16 (setq RCYL 0.20)
17 (setq CYLCOL1 "CYAN")
18 (setq CYLCOL2 "YELLOW")
19 (setq PTCOL "RED")
20 (setq RPT 1)
21 (setq ICOL "YELLOW")
22 (setq RI 1.5)
23 (atom PT1 RPT PTCOL)
24 (atom PT2 RPT PTCOL)
25 (atom PT3 RPT PTCOL)
26 (atom PT4 RPT PTCOL)
27 (atom PT5 RPT PTCOL)
28 (atom PT6 RPT PTCOL)
29 (atom PT7 RPT PTCOL)
30 (atom PT8 RPT PTCOL)
31 (atom PT9 RPT PTCOL)
32 (atom PT10 RPT PTCOL)
33 (atom PT11 RPT PTCOL)
34 (atom PT12 RPT PTCOL)
35 (atom PT13 RPT PTCOL)
36 (cyl PT1 PT2 RPT RPT RCYL CYLCOL1)
37 (cyl PT1 PT4 RPT RPT RCYL CYLCOL1)
38 (cyl PT1 PT10 RPT RPT RCYL CYLCOL1)
39 (cyl PT2 PT3 RPT RPT RCYL CYLCOL1)
40 (cyl PT2 PT5 RPT RPT RCYL CYLCOL1)
41 (cyl PT2 PT10 RPT RPT RCYL CYLCOL1)
42 (cyl PT2 PT11 RPT RPT RCYL CYLCOL1)
43 (cyl PT3 PT6 RPT RPT RCYL CYLCOL1)
44
45 (cyl PT3 PT11 RPT RPT RCYL CYLCOL1)
46 (cyl PT4 PT5 RPT RPT RCYL CYLCOL1)
47 (cyl PT4 PT7 RPT RPT RCYL CYLCOL1)
48 (cyl PT4 PT10 RPT RPT RCYL CYLCOL1)
49 (cyl PT4 PT12 RPT RPT RCYL CYLCOL1)
50 (cyl PT5 PT6 RPT RPT RCYL CYLCOL1)
51 (cyl PT5 PT8 RPT RPT RCYL CYLCOL1)
52 (cyl PT5 PT10 RPT RPT RCYL CYLCOL1)
53 (cyl PT5 PT11 RPT RPT RCYL CYLCOL1)
54 (cyl PT5 PT12 RPT RPT RCYL CYLCOL1)
55 (cyl PT5 PT13 RPT RPT RCYL CYLCOL1)
56 (cyl PT6 PT9 RPT RPT RCYL CYLCOL1)
57 (cyl PT6 PT11 RPT RPT RCYL CYLCOL1)
58 (cyl PT6 PT13 RPT RPT RCYL CYLCOL1)
59 (cyl PT7 PT8 RPT RPT RCYL CYLCOL1)
60 (cyl PT7 PT12 RPT RPT RCYL CYLCOL1)
61 (cyl PT8 PT9 RPT RPT RCYL CYLCOL1)
62 (cyl PT8 PT12 RPT RPT RCYL CYLCOL1)
63 (cyl PT8 PT13 RPT RPT RCYL CYLCOL1)
64 (cyl PT9 PT13 RPT RPT RCYL CYLCOL1)
65 (cyl PT10 PT11 RPT RPT RCYL CYLCOL1)
66 (cyl PT10 PT12 RPT RPT RCYL CYLCOL1)
67 (cyl PT11 PT13 RPT RPT RCYL CYLCOL1)
68 (cyl PT12 PT13 RPT RPT RCYL CYLCOL1)
69 (command "redraw")
70 )
```

Figure 4. Molecule definition file for a cluster of 13 platinum atoms

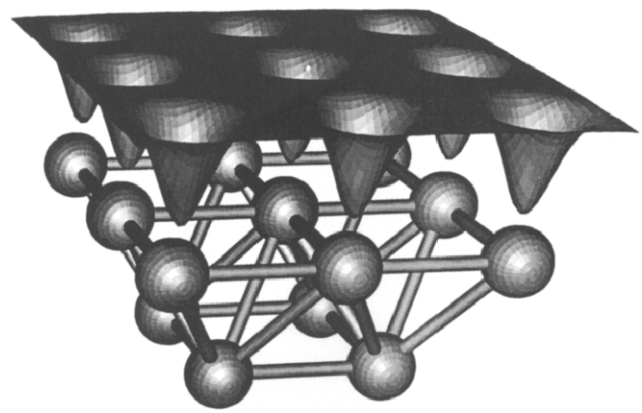

Figure 5. Postscript black-and-white version of Color Plate 2

listing in Figure 2. The cluster is to be shown, for example, with part of a quantum-chemically calculated potential energy surface. Drawing surfaces given by a list of (x,y,z) values is already implemented in AutoCad and no additional programming is needed. For the grid superimposed here the AutoCad standard command 3DMESH was used. 3DMESH requires as parameters the number of points in the x- and y-directions and the x-, y- and z-values of all points. Color Plate 2 (color) and Figure 5 (black and white) show the cluster with the corresponding cut of the potential energy surface.

No examples of calott models are provided since it is obvious that they can be created by using larger atomic radii and omitting the bond sticks.

SUMMARY

It is possible to produce high-quality pictures and printouts of molecular models with standard CAD software running on simple personal computer-based equipment. This is an alternative to taking off-screen photographs. Little programming effort is necessary because all of the low-level work is already implemented in the CAD program and CAD software is programmable. It is further possible to produce highly customized pictures, which on most other software would require substantial reprogramming.

APPENDIX

In this appendix some technical information is collected that might be of use for those who try to use AutoCad and AutoShade to produce pictures similar to the ones presented here:

(1) If the AutoCad screen has the dimensions of an A4 sheet of paper and the center of the molecule is in the middle of the screen, the following AutoLisp settings might be tried: In menu Camera Position: right 260°, up 35°, distance 55, lens 25; menu Shading Model: ambient 0.3, diffuse 0.5, specular 0.3. For all other settings default values are convenient.

(2) AutoCad and AutoShade are also available in special 386 versions for IBM-compatible personal computers having a 80386 processor. If speed is a problem, AutoShade-386 is primarily recommended because the AutoShade step is much more time consuming than the AutoCad step. This step is speeded up by a factor of about 10 by AutoShade-386.

(3) The time to produce our two examples was about 40 minutes each, from processing the input file to creating the postscript file.

(4) Many color postscript printers offer much higher quality than the PaintJet printer. However, their prices as well as the costs per page are presently quite high.

(5) An advantage of the postscript printing language is the possibility to introduce modifications by editing the postscript file before sending it to the printer. If, for example, a poster in format A2 is desired it can be assembled from A4 format sheets created by AutoShade by printing 4 pages that have the additional line

```
-x -y translate ; 2 2 scale
```

inserted at the beginning; x and y take the values (0,0), (500,0), (0,700), and (500,700), respectively.

(6) If black-and-white graphs are to be produced the quality of the hard copy is often better if AutoShade already deals with only one color, instead of letting the hard copy device translate color information into shades of gray.

(7) AutoShade can also produce color separations, which is often an advantage for publication purposes.

(8) If no postscript device is available, software like Ultrascript[6] can be used to print postscript files on many printers (including the PaintJet printer) at the cost of speed.

(9) The C D software described here also supports the creation of animated pictures, i.e., to visualize molecular vibrations. This, however, is beyond the scope of this article.

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NOTE ADDED IN PROOF

After preparation of this article, new versions of AutoCad and AutoShade became available. AutoCad version 11.0 supports solid modeling in a better way and is able to precompile LISP functions that should offer some speed advantage. AutoShade version 2.0 supports the so-called Renderman interface, which means that surfaces and materials are defined not only by their color but also by texture, transparency and other attributes. This offers some nice possibilities of distinguishing different kinds of atoms. It is also possible, for example, to enclose a ball and stick model inside a transparent calott model to get the advantages of both representations.