

# ADFview

# Tutorial and

# Reference Manual

ADF Program System  
Release 2002.02

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June 20, 2002

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## INTRODUCTION

ADFview is a small utility program, which provides some basic volume visualization tools. It will enable ADF users to visualize their results: SCF densities, orbitals, electrostatic potentials, and any other property that is available as a scalar value over a grid.

The documentation of ADFview consists of two main sections.

The first part is a very basic hands-on tutorial. Its purpose is to help you create some pictures, and to have a simple and fast tour of the main features of the utility. We estimate that you should be able to finish this section including the hands-on activities within 30 minutes.

The second part explains in detail all possible options, buttons and so on. This material is mainly included as a reference. We hope that the utility is easy to use, and that the options, together with the help information popping up, will not require you to use the reference manual.

At this point in time, ADFview is still under development and is being tested. It is now released as a first version as a service to our customers. Your suggestions and bug reports are valuable to us for making an improved and extended next release available as soon as possible.

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of ADFview, but do not contain personal information.

You can enable this by setting the global environment variable `SCMERRORMAIL`, for example in your login script:

```
SCMERRORMAIL=yourmail@your.institute.com
export SCMERRORMAIL
```

This will ensure that the bug report will be sent back to us, and also to the mail address you specify. Thus you can see exactly what kind of information you are mailing to us. If you do not want to receive a copy yourself, please set `SCMERRORMAIL` to `'errors@scm.com'`, without quotes.

Your comments and bug reports are very welcome. Please send them to `support@scm.com`.

# TUTORIAL

This tutorial will help you to:

- perform a simple ADF calculation on a water molecule
- generate some volume properties (densities, orbitals and electrostatic potential)
- visualize these volume properties in a variety of ways.

We will assume that you have installed the ADF package on your machine, and that you are familiar with running ADF jobs.

On all UNIX platforms, including Mac OS X, ADFview is an XWindow program. Your environment should have been set up correctly to run such programs. In particular, you need to make sure that your DISPLAY environment variable has been set properly.

You can test this easily by starting a simple X program from your shell:

```
xclock &
```

Assuming the xclock program is in your \$PATH, a small window should appear with the image of a clock. If not, please consult your local system administrator for additional help. Typical problems have to do with your DISPLAY variable, and with security issues when trying to connect to the X server.

ADFview is available for all platforms for which ADF is available.

## STEP 1: PERFORM AN ADF CALCULATION

We start with a simple geometry optimization of the water molecule.

### Create a subdirectory for this tutorial

```
mkdir $HOME/tutorial  
cd $HOME/tutorial
```

## Create a run script

Use an editor to make a file 'run' with the following contents:

```
$ADFBIN/adf -n 1 <<eor
```

```
atoms
```

```
O 0 0 0
```

```
H 1 1 0
```

```
H -1 1 0
```

```
end
```

```
basis
```

```
end
```

```
geometry
```

```
end
```

```
eor
```

## Perform the ADF calculation

Enter the following commands:

```
chmod u+x run  
./run >run.out
```

After ADF has finished you can examine the output file (run.out) to verify correct execution.

In the current directory, ADF has created a file with the name 'TAPE21'. This file contains detailed results of the calculation, including orbitals, densities, and so on.

## STEP 2: CALCULATE VOLUME PROPERTIES ON A GRID

Next we need to calculate the numerical values of the volume properties we want to visualize on a grid. For this tutorial we will use a grid of medium quality, which will also be good enough for many real applications.

The calculations in this step are performed using the program densf (release 2002.02). It requires only one line of input to get a grid of medium quality. The volume properties

selected by default by densf will work fine for this tutorial (SCF density, sum of fragment density, for each symmetry the HOMO-1, HOMO, LUMO and LUMO+1 orbitals, and the electrostatic potential).

Enter the following command:

```
$ADFBIN/densf -n 1 <<eor  
grid medium  
eor
```

You will have to wait a minute or so for the program to finish.

You should now have a file called TAPE41. This file contains the data to be visualized on a grid, and has just been generated by densf.

### STEP 3: VISUALIZE THE RESULTS

#### Start ADFview

Enter the following command:

```
$ADFBIN/adfview TAPE41
```

A new window will be created on your display. The upper part of this window contains a picture, if available. The lower part contains the controls you use to tell ADFview what to do.

Immediately after starting, ADFview will scan TAPE41 as specified on the command line. Next it will load some volume properties from it, and it will start calculating and displaying an image. Please be patient, and let the program continue the calculations until the picture has been created in the best possible quality.

In the lower right corner of the ADFview window you can see if the picture is complete. The number in parentheses is an indication of the quality of the picture being calculated, with 1 being the best quality. The percentage value is the part of the calculations completed.

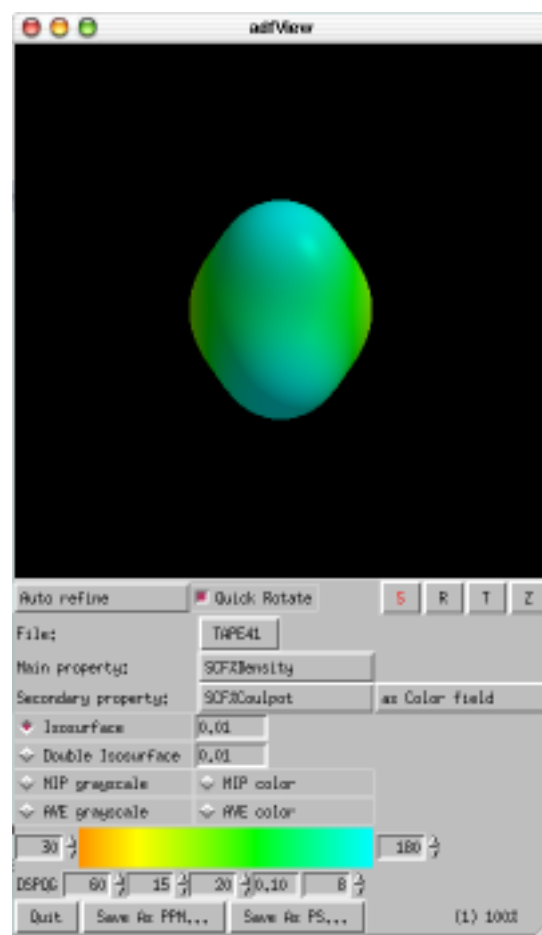


Fig. 1 Isodensity surface with Coulomb potential

This image is an isosurface of the SCF density, and has been colored with the electrostatic potential. Later in this tutorial we will show you how to generate different pictures. The isosurface value is 0.01. You can change that by simply changing the number to the right of 'Isosurface'.

## Play around with the color range

You can change the color range used to indicate different values of the electrostatic potential. The entire range of the electrostatic potential values is mapped on the color range visible in the horizontal color bar. You can change this bar:

- Click on the little arrows next to the color bar

The image as well as the color bar will update immediately. You can also change the color range by changing the numbers on the left and right side of the bar:

- Select the right number by double-clicking on it.
- Type a new value (500)
- Press the Return key

Again, the picture and color bar will update immediately.

## Rotate the image

The following instructions assume you are using a three-button mouse. If you have a mouse with one or two buttons, check the description of the S, R, T, and Z buttons in the reference manual to learn how to achieve the same effects.

- Click in the picture and hold down the right mouse button

The picture will change into a simple cube.

- Move the mouse around (still pressing the right mouse button!)

The picture of the cube will rotate.

- Release the mouse button

The cube will disappear, and ADFview will recalculate the isosurface of the density in the new orientation.

Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you were rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle), the rotation will be around an axis perpendicular to the screen.

## **Zoom the image**

- Press and hold the control key, click in the picture and hold down the right mouse button

The picture will change to a simple cube.

- Move the mouse to the right (still pressing the right mouse button and control key!)

As the picture of the cube shows, you will zoom in.

- Move the mouse to the left (still pressing the right mouse button and control key!)

You will zoom out.

- Release the mouse button

The cube will disappear, and ADFview will recalculate the isosurface of the density with the new zoom settings.

## **Translate the image**

- Click in the picture using the middle mouse button, and hold down the mouse button
- Drag the mouse in some direction

The image (temporarily replaced by the picture of the cube) will be translated following the mouse.

## **Remove electrostatic potential coloring**

- Click on 'as Color Field' and hold the mouse button down

A menu will appear. This menu tells you how ADFview is using the 'secondary property' selected (currently the electrostatic potential).

- Select the '- not used -' entry

A simple grayscale picture of the isosurface of the SCF density will replace the image.

## View an orbital

- Click on 'SCF%Density' and hold the mouse button down

A menu will appear. This menu lists all volume properties available on TAPE41.

- Select the 'SCF\_A1%2' entry

This is the 2nd orbital in the A1 representation, in this case the HOMO within the A1 representation.

The image will change but is not quite optimal. So:

- Click on 'Double Isosurface'
- Change the number next to it from 0.01 to 0.04

Now a double isosurface should appear. One isosurface corresponds to an isosurface value of 0.04. The other one with a different color corresponds to a value of -0.04. The color on the left side of the color bar is used for the negative isosurface, the color on the right side of the color bar is used for the positive isosurface.

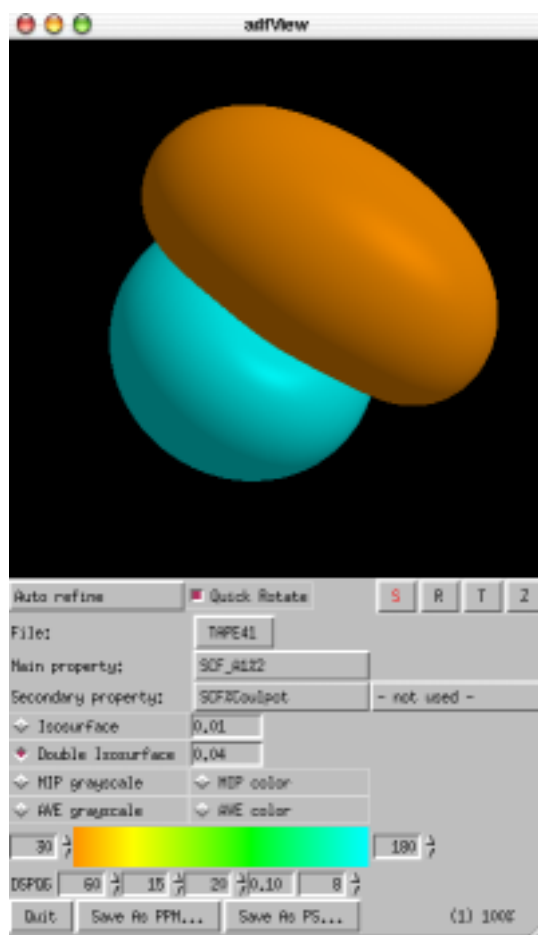


Fig. 2 Double isosurface for HOMO orbital.

## View a difference field

- Select 'SCF%density' as main property
- Select 'SumFrag%Density' as secondary property
- Change '- not used -' to 'as Difference field'
- Select the 'Double Isosurface' option
- Set the number next to 'Double Isosurface' to 0.004

These isosurfaces show the difference density between the final SCF density, and the sum of fragments density. Loosely speaking, it shows you how the density changes when building the water molecule from the atomic fragments.

A positive value means that the main property is larger than the secondary property.

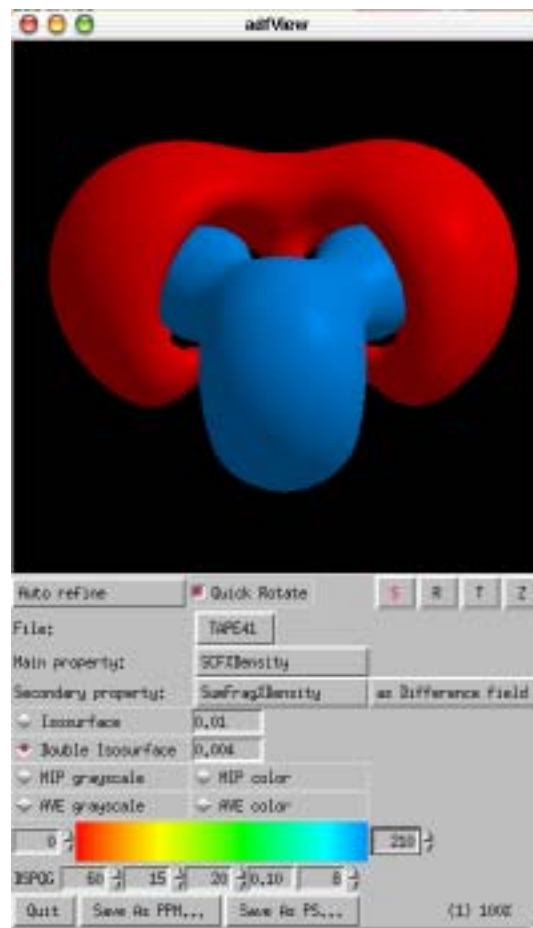


Fig. 3 Deformation density.

## View the positive or negative part of a difference field

- Change 'as Difference field' to 'as Neg Diff field'
- Select Isosurface
- Change the isosurface value to 0.004

Now you are viewing the negative part of the difference between the SCF density and the sum of fragments density. The values have been negated to get a positive field.

- Change 'as Neg Diff field' to 'as Pos Diff field'

Now you are viewing the positive part of the same difference field.

## View a MIP grayscale image of the density

- Select 'SCF%Density' as main property
- Select '- not used -' as option with the secondary property
- Select the 'MIP grayscale' mode

Now you see an image that looks very much like a 'Röntgen picture' of the molecule. You can clearly see the oxygen atom as well as the two hydrogen atoms.

MIP stands for Maximum Intensity Projection. Thus, the image is constructed by sending 'rays' through the data set, and the maximum value encountered determines the intensity at that point of the image.

The nice thing about these pictures is that you can see most of the features in your molecule. The problem is that you do not get a feeling of the three-dimensional structure of it. Of course you can still rotate, and 'take the Röntgen picture from a different angle'.

## View MIP color image

- Select the 'MIP color' mode

You will get a similar picture in color.

By playing with the color scale (the horizontal color bar again) you can choose colors which make the features you are interested in better visible. By choosing a large color range (for example from 0 to 1000) you will see many details but in a very busy picture.

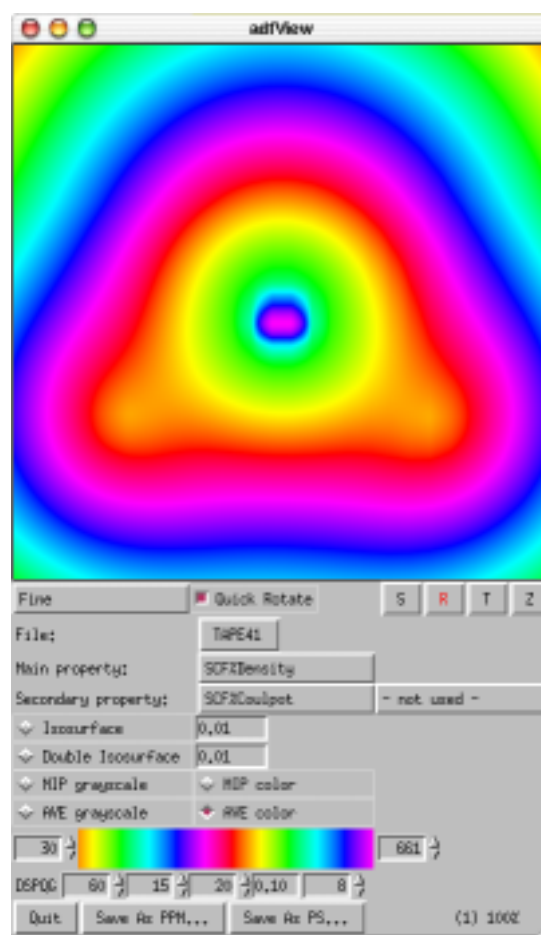


Fig. 4 AVE (like MIP) density image shows Oxygen and Hydrogen atoms.

## **Save picture to file**

- Click the 'Save As PS...' button

A standard file select dialog box will appear.

Use it to tell ADFview where to save a postscript file with a screen shot of the current picture.

# REFERENCE MANUAL

## STARTING ADFVIEW

If you have installed the ADF package correctly, ADFview is located in \$ADFBIN.

If \$ADFBIN is included in your PATH environment variable, you can start the ADFview program with the following command:

```
adfview [filename]
```

The filename is optional.

## DATA FILE

The data file is a KF file, which is the ADF binary file format. The Utilities document describes the KF utilities that can be used to manipulate these KF files (e.g. to convert it into an ASCII format and vice versa).

The data file is divided into sections containing the property values on a grid, for all properties you have selected in densf. Currently only scalar fields are supported. The data file also contains a specification of the grid used.

ADFview is not restricted to the properties calculated by densf. You can use the program to visualize any kind of scalar field. Just calculate its values on the grid, and save the result in a KF variable in the format used by densf. The name given to the KF-variable will automatically be added to the property pull-down menus within ADFview.

If you have specified a filename at the invocation of ADFview that file will be used as data file. Alternatively, you may click on the button 'Click to select file'. A standard file select dialog box will appear, and you will be able to select the data file you want to use. The name of the button will change into the name of the file being used.

If you want to use a different file without restarting ADFview, just click on the name of the file again, and you will again be able to select a data file.

## MAIN PROPERTY

The main property is one of the data fields available on the selected data file, and will be used to generate isosurfaces and the MIP and AVE pictures.

You can select any property available on the data file using the pull-down menu.

## **SECONDARY PROPERTY**

The secondary property is also one of the data fields available on the file. You can select it with the pull-down menu.

## **SECONDARY OPTIONS**

The pull-down menu to the right of the secondary property pull-down menu determines what the secondary property is used for.

### **- not used -**

The secondary property will not be used at all.

### **as Color field**

The secondary property will be used to paint the main isosurface with colors determined by the secondary property. The range of colors used corresponds with the horizontal color bar, and is mapped to the range of scalar values that occur in the secondary field.

Typical use is to display the values of the electrostatic potential as different colors across an iso-density surface.

### **as Difference field**

The secondary field will be subtracted from the main field.

For example, use this option to see the differences in density between the final SCF density and the sum of fragments density. Another application might be to visualize the difference between alpha and beta spin densities.

A more advanced use would be to view changes that result from using a different basis set or Hamiltonian. To do this you would need to combine the results from two different densf runs. This is easy to do using the KF utilities.

### **as Pos Diff field**

This option is similar to 'as Difference field', but this time only the positive part of the difference is retained. The negative part of the difference has been set to zero.

Use this option to clean up a complex situation, or in combination with MIP or AVE. These visualization modes can only handle positive fields.

### **as Neg Diff field**

This option is similar to 'as Difference field', but this time only the negative part of the difference is retained, with inverted sign. The positive part of the difference has been set to zero.

Use this option to clean up a complex situation, or in combination with MIP or AVE. These visualization modes can only handle positive fields.

## **VISUALIZATION MODES**

### **Isosurface**

Construct an isosurface and show it, using shading and reflections based on the (numerical) gradient. Only one isosurface is visible, no colors.

The isosurface value used is the number in the box to the right of the Isosurface mode box. You may enter any numerical value you like, including negative values.

### **Isosurface with Color field**

When an isosurface is combined with a secondary 'Color field', the same surface is displayed, but painted with colors based on the secondary field. The color range used is determined by the horizontal color bar.

## **Double Isosurface**

Two isosurfaces are constructed: one for the value entered, and one for the opposite value. The extreme colors of the horizontal color bar are used to distinguish the two surfaces. Shading and reflections are done the same as with a single isosurface.

Since color is already being used to distinguish between the two surfaces, there is no possibility to use a color field.

## **MIP grayscale / color**

The Maximum Intensity Projection images are a nice way to have a look at your molecule: you will be able to see many details that would be difficult to view using only an isosurface.

The construction of MIP images is simple but expensive. From your eye, a ray is cast through the data set. The maximum intensity of the data set along this ray determines the intensity or color. For coloring, the horizontal color bar is used again.

Most fields used in combination with ADF have very large differences in numerical values around nuclei and the rest of space. So ADFview always takes a logarithm of the field values before calculating a MIP image. For that reason, only positive fields can be displayed.

## **AVE grayscale / color**

The AVErage intensity projection images are similar to MIP images.

The construction is as for a MIP image, but now the average value along the ray is used. In this case also the logarithm of the field value is used.

## **MOUSE INTERACTION**

Following is a description how to rotate, translate or zoom the picture. We assume the Standard mouse mode is active, as described later. To ensure this, click on the S button just below the picture.

If you have a mouse with only one button, this button is always equivalent to the 'left' button.

## **Rotate the image**

Click in the window, somewhere on the picture shown, and hold down the right mouse button. The picture will change to a simple cube. If you move the mouse around within the window, the picture will rotate. When you release the mouse button, the cube will disappear and ADFview will recalculate the isosurface of the density in the new orientation.

Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you are rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle) the rotation will be around an axis perpendicular to the screen.

Alternatively, you may use the left mouse button together with the shift key.

## **Zoom the image**

Click in the picture using the right mouse button while holding the control key, and move the mouse to the right: you will zoom in. Moving the mouse to the left (with the right mouse button and control key pressed down) will zoom out.

Alternatively, you may use the left mouse button together with the control and shift keys.

## **Translate the image**

Click in the picture using the middle mouse button and drag the mouse in some direction. The image will be translated following the mouse.

Alternatively, you may use the left mouse button together with the control key.

## **The SRTZ mouse mode buttons**

You may change the reaction to mouse clicks completely by changing the mouse mode using the S, R, T, or Z buttons.

The S button is the Standard mouse mode. Mouse interaction is exactly as described before. If you want to return from any of the other modes, just press the S button again.

If you click the R button, the Rotate mode is active. Dragging with the left mouse button will rotate the image.

If you click the T button, the Translate mode is active. Dragging with the left mouse button will translate the image.

If you click the Z button, the Zoom mode is active. Dragging with the left mouse button will zoom the image.

The mouse mode will change only by clicking in one of the S, R, T, or Z buttons.

## **Resize window**

You can resize the window as usual, by grabbing the lower right corner of the window with your mouse, and dragging it. You may have to use a different technique, depending on the window manager you are using.

The picture area will enlarge as much as possible, and the picture will be rescaled.

A bigger picture will take more time to calculate and to draw, since more pixels need to be handled.

If you need a high-resolution picture you can use this technique: make the window big, save the picture in a file, import that file into your graphics program, and finally rescale the image to get an image with a resolution better than the screen resolution.

## **COLOR RANGE**

Using the horizontal color bar, you can change the color range used for different images. Change the number on the left or right by selecting and typing the new number, and pressing return. Alternatively, you can change the numbers by clicking on the arrows next to the numbers.

The color range is used to visualize the value of a color field on a single isosurface, or to display the value of the field in a MIP or AVE picture.

The extreme colors (left and right side) are used to distinguish the two isosurfaces in case the double isosurface option is active.

## **COMMAND BUTTONS**

Quit: quits ADFview.

Save As PPM...: save the current picture in ppm format. This format is a color bitmap format and can be handled by many image manipulation programs to convert it into your preferred graphic format. Since the bitmap contains all pixels in the picture, the resulting quality is better when you increase the size of your window.

Save As PS...: save the current picture in postscript format. Again, you can get a better quality by increasing the size of your window.

## **EFFICIENCY AND QUALITY**

The pull-down menu just below the picture determines how the picture quality is improved. It has effect only on the calculation of the displayed picture. Another important factor is of course the density of the grid used as input for ADFview.

### **Simple Cube**

The most basic picture is a picture of a cube only. This is very fast, and contains only information about the orientation and scaling of the data set.

### **Coarse**

This will produce the real picture but in a very coarse resolution: the image is calculated in block of 16 x 16 pixels at a time.

### **Medium**

This will produce an acceptable but still low-quality image. The image is calculated in blocks of 4 x 4 pixels at a time.

### **Fine**

This will produce a picture at the best possible quality given the current data set and grid quality. The color of each pixel in the image is calculated individually. This gives the best quality, but may require some patience.

## **Auto refine**

Starts the display with a coarse picture, and updates the quality if you are not doing anything. The updating will continue until the picture has been recalculated at the best possible quality ('Fine').

## **Quick Rotate**

This check box determines what to do when rotating, zooming or translating: temporarily replace the picture with the picture of a cube, or continue with the current picture.

Displaying the cube while rotating and so on of course greatly improves the interactive response.

## **ISOSURFACE PROPERTIES**

The line with 'DSPQG' in front of it determines some properties of the isosurfaces generated. The first number corresponds to the D, the next one to the S, and so on.

### **D: amount of directed light.**

100 means only directed light, 0 means only diffuse light.

### **S: amount of specular reflections**

These are the 'highlights' reflecting from the surface.  
100 means specular reflections only, 0 means no reflections.

### **P: power of the specular reflections.**

This determines the 'size' of the bright reflecting spots.

### **Q: quality setting.**

To speed up things, ADFview uses an algorithm where the isosurface is calculated first in a coarse resolution. When all four corners of a square in this resolution have the surface

at the same distance, ADFview uses that value for the entire square. A great speed up is achieved for surfaces parallel to the screen, and for empty space.

The quality setting is the numerical threshold on these distances to determine if they are equal.

Increasing the value from the default 0.10 speeds up the algorithm at the expense of artifacts, especially with surfaces with small details or disconnected surfaces.

Reducing the value slows things down but removes any artifacts introduced. Setting the value to a negative number ensures that no approximations in this respect are used.

### **G: gamma value.**

This determines the overall 'contrast' of the picture. Adjust to your taste.

## **STATUS FIELD**

In the lower right corner you will see a status field. This informs the user what ADFview is currently doing.

The percentage number is the percentage of the image currently being calculated which has been completed. Thus, 100% shows you that the calculation is complete.

The number within parentheses shows the current resolution. If the number is  $n$ , the picture has been calculated with blocks of  $n \times n$  pixels. Thus, (1) indicates that the picture being calculated is a picture at the highest possible resolution (corresponding to the 'Fine' option in the pull-down menu).