ELSEVIER

Eadfrith: A molecular rendering program for Silicon Graphics workstations

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Eadfrith was written to provide the rapid display of molecules, so that they can be interactively rotated, translated, and scaled, and then rendered in a manner suitable for photography or other high-quality output methods. The program provides support for the display of transparency, electrostatic effects, and the normal vibrational modes of molecules. The compiled version for Silicon Graphics machines is freely available over the World-Wide Web. Eadfrith reads the structures from files in MacroModel format. The aim of the program is to provide a way to display molecular structures quickly and to produce high-quality pictures. Consequently, image-saving routines are not included, and standard utilities must be used in conjunction with Eadfrith to save the images to disk.

Keywords: graphics, molecular structure, electrostatics

INTRODUCTION

MacroModel[1] is the principal molecular modeling program in our laboratory, but it is not ideal for all applications. It is a complex program that presents the user with a large number of options to utilize the wide range of functionality it contains. We wanted a program that would display molecules in a clear way, and produce pictures that are suitable for papers and posters, but which was as simple as possible. Eadfrith was written in response to this need.

Eadfrith has three main functions:

1. To provide wireframe models of molecules, which can be interactively rotated, translated, and scaled
2. To provide high-quality pictures of molecules that are suitable for making posters or including in publications
3. To animate the normal modes and other movements of molecules

The program is written in Fortran and uses the GL library. The executable is freely available over the World-Wide Web. The program has been tested on a variety of Indy, Indigo II, Indigo, and Personal Iris workstations, using either IRIX 4 or IRIX 5 operating systems. The best pictures are obtained using machines with 24-bit color, but the program runs on machines with less powerful graphics. The quality of the rendered pictures depends just on the number of bit planes, and not on other aspects of a machine's graphical capability.

DESCRIPTION OF PROGRAM

The program is invoked by typing **eadfrith filename,** where filename is the name of a file containing a MacroModel format molecule. The user is then presented with a menu (Table 1). A variety of options to control the picture are available and are described below. The simplest possibility is just to press the Return key. A wireframe picture of the molecule will then be drawn, which may be scaled, moved, and rotated using the mouse keys (Figure 1).

Once a suitable orientation has been chosen, the molecule can be rendered by pressing the space bar. The rendered image can then be captured using a utility such as *scrsave* or *imgsnap*. Eadfrith does not write image files directly. The Esc key can be used to stop the program at any time.

APPEARANCE OF WINDOW

The size of the window can be controlled using *Option C*. This can be specified with particular dimensions, adjusted interactively when the window is first displayed, or set to fill the whole screen. The color of the background is controlled by *Option E*.

WIREFRAME MODEL

Eadfrith begins by drawing a wireframe model of the molecule. Usually, this will be in the orientation of the data file,

Color Plates for this article are on page 91.

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Received 4 January 1996; revised 20 February 1996; accepted 27 February 1996.

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0263-7855/96/$15.00
PII S0263-7855(96)00021-5

Table 1. Eadfrith options

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************************************************
************************************************
*************        EADFRITH          *************
************************************************
************* JONATHAN GOODMAN (1995) *************
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************************************************

Use ESC key to exit, SPACE to render
LEFTMOUSE to enlarge,
MIDDLEMOUSE to rotate, RIGHTMOUSE to move.

Options:
(A)         Radii:          1.000000
(B)         Bond Option:            0
(C)         Full screen picture
(D)         Full contrast
(E)         Background colour (RGB):  0  0  0
(F)         New Orientation
(G)         No NMA
(H)         Colour option           0
            Reading Colours
(I)         No Initial Depth Cue
(J)         Line Width:             1
(K)         Ambient Light  0.5000000
(L)         Bond radius  0.1000000
(*)         Quit
Enter a letter, then RETURN, to alter options
or press RETURN to continue
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but *Option F* allows the orientation of the last molecule to be used instead. A file called *.Eadfrith__Options* is written to the current directory to store this information. The depth cueing of the wireframe model is controlled by *Option I.* This does not affect the final rendered picture. The width of the lines that make up the wireframe model can be varied using *Option J.*

RENDERED MODEL

The size of the spheres in the rendered model can be altered, to give ball-and-stick models, CPK models, or anything in between. The van der Waals radius of each atom is multiplied by the factor entered using *Option A.* The atoms are colored in a standard way, or by colors read from a file (see Data Files) or by their electrostatic properties (see Electrostatic Properties). The choice is made using *Option H.* Bonds can be colored by bond order or by taking their color from the atoms they join. This is decided by *Option B.*

The rendered molecules are depth cued, and *Option D* controls the contrast in the rendered picture. Full contrast means that the nearest atoms are as bright as possible, and the most distant atoms are depth-cued almost into the background. Reduced contrast lessens the effect of depth-cueing, and may make the picture more suitable to be photographed.

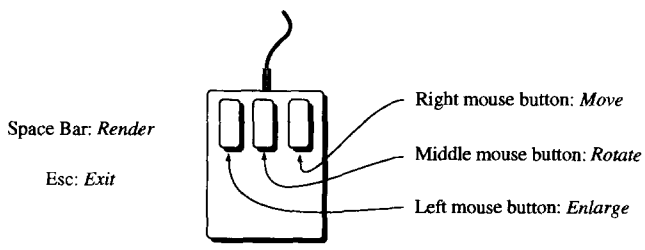

Figure 1. Control keys for Eadfrith.

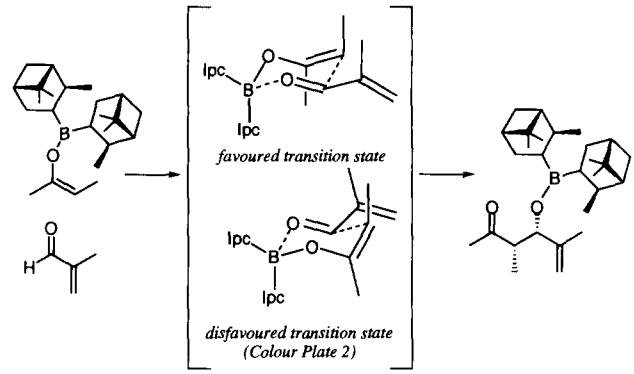

Figure 2. A boron-mediated aldol reaction.

The ratio of ambient to directional light in the rendered figure is chosen using *Option K.* A value of 1.0 will give 100% ambient light, and the molecule will appear rather flat. A value of zero will give each sphere a dark outline, as no light is reflected back toward the viewer. An intermediate value usually gives the best results.

The rendering algorithms use some of the procedures of the Silicon Graphics GL library, which are explained in Silicon Graphics documentation.

TRANSPARENCY

Transparency is introduced by editing a MacroModel file, to introduce atom types with numbers exceeding 100. These atoms are transparent. Their colors and degree of transparency are controlled by the *Eadfrith__ Atom__ Types* (see Data Files).

ELECTROSTATIC PROPERTIES

If electrostatic color options are chosen (*Option H,* 2 or 3), then Eadfrith will expect to find a file *filename.ele* as well as *filename.* This file must contain a list of atom-centered charges, in the same order as the atoms in the data file. Option 2 gives continuously shaded colors. Option 3 gives stepped colors, with user-definable boundaries. Once the picture is complete, the maximum and minimum values of the potential are printed. This may be used as a guide to where the boundaries should be chosen.

OPTION G: NORMAL MODE ANALYSIS

Option G was designed to animate normal mode analyses, but may also be used to display other molecular motions. The input required is a MacroModel file containing a series of structures, corresponding to different distortions of the molecule along one of its normal modes. Such a series of files may be created using the outputs of many molecular orbital programs. The program asks how many of the structures should be read, and what delay there should be between them. A value of 10 for the delay is often a good choice. The program will read in all the structures together, and then flip between them when the mouse is moved with no buttons pressed. Pressing the mouse buttons has the usual effect.

DATA FILES

The program looks for two files: *Eadfrith__Atom__Types* and *Eadfrith__Mmod__Types*. It looks first in the directory from which the program is being run, then in the user's home directory, then in the directory defined by the environment variable EADFRITH__HOME. If it cannot find both the files by searching these three places, the program will stop with an error message.

The *Eadfrith__Atom__Types* file contains comments and then a list of atom types. Each line contains first an atomic number, then the red, green, and blue components of the color of such an atom (0–255), and then the atomic radius. Some atomic numbers over 100 are included. These are transparent atoms, and they have an extra number corresponding to their transparency. A transparency of 0 is invisible, whilst a transparency of 1 is opaque. The *Eadfrith__Mmod__Types* file contains a list of MacroModel atom types and their colors.

EXAMPLES OF EADFRITH OUTPUT

Two examples of Eadfrith output are given in Color Plates 1 and 2. Color Plate 1 is an image of a DNA base pair, with its surface colored by the electrostatic potential at each point. Blue represents the most negative regions, and red the most positive. The structure was obtained by molecular mechanics minimization with the MM2 force field,[2] and the electrostatic potential was calculated from electrostatic potential-derived atom-centered charges, using a single-point AM1 calculation[3] with MOPAC6.[4] The same structure is also illustrated as a ball-and-stick model.

Color Plate 2 shows the transition state for a boron-mediated aldol reaction (Figure 2), calculated using MacroModel. The transition state shown leads to the minor product, due to the steric interaction highlighted by transparent yellow spheres. Eadfrith pictures have also been used in a variety of publications.[5–9]

OBTAINING THE PROGRAM

The executable for Eadfrith may be freely distributed, provided this article is cited whenever its pictures are used. The source code is not available. The executable (for Silicon Graphics machines) may be obtained from the Cambridge WWW server (http://www.ch.cam.ac.uk/). The latest news about the program and the executable are available at URL: http://www.ch.cam.ac.uk/MMRG/eadfrith.html. An example normal modes analysis file is also available from this page.

ACKNOWLEDGMENTS

The Royal Society, the Cambridge Centre for Molecular Recognition, and Silicon Graphics Computer Systems are thanked for their support of this work.

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