



Figure 8.

$$R_{1s} = 2\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a}$$

$$R_{2s} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a}\right)^{3/2} \left(1 - \frac{Zr}{2a}\right) e^{-Zr/2a}$$

Figure 6 shows a three-dimensional plot of the 1s orbital, and Figure 7 shows a similar plot for the 2s orbital. The wave function dips somewhat below the zero plane in the 2s orbital, but it is not easily seen on this plot. Figure 8 shows a plot of the square of the 2s wave function with the z axis greatly expanded, and the rises and falls of the probability function are clearly seen. These types of plot (which are even more striking in color on the terminal screen) can be easily generated, thus providing the opportunity for visual interpretation of a function's meaning.

In summary: Mathematica is an extremely capable software system that can be used for many varied tasks in the general area of mathematics. Its strength lies in its ability to perform symbolic algebraic and other mathematical manipulations, coupled with the ability to provide graphical output. The package has capabilities in statistical analysis and general graphical production, but other packages can also do these tasks well. Mathematica is costly, and it requires a lot of memory and disk space to implement. It does take time to learn how to use the system, compared to other typical MS-DOS software packages. The input mechanism is somewhat cumbersome compared to other software packages. However, Mathematica shines where it can perform functions not easily available elsewhere that could be of great utility to chemists, especially in symbolic mathematics. The system couples with the outside world through its interfacing routines, and it can be used to tackle problems using its own language. Overall, Mathematica is a superior software product if its strengths match well with your needs.

REFERENCES AND NOTES

- (1) Mathematica is available from Wolfram Research, Inc., 100 Trade Center Drive, Champaign, IL 61820-7237. The price varies widely depending on hardware platform and license specifics. The list price for single-user systems of the commercial and government version appropriate for a 386-based PC system under MS-DOS is \$595 (\$475 Educational) for the Standard version and \$895 (\$725 Educational) for the Enhanced version. The same prices apply to the Macintosh versions. For the Microsoft Windows version for 386-based PC systems, it is \$995 (\$795 Educational). Mathematica is available to students for \$175 for MS-DOS, Microsoft Windows, and Macintosh machines.
- (2) Cooper, R.; Casanova, J. Two-dimensional atomic and molecular orbital displays using Mathematica. *J. Chem. Educ.* **1991**, *68*, 487-488.
- (3) Levine, I. *Quantum Chemistry*, 3rd ed.; Allyn and Bacon, Inc.: Boston, MA, 1983; p 121.

Edifice¹

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This program is essentially a database manager with calculation and graphing capabilities. In its delivered form, it is a system for setting up to use the data from environmental methods of determination to produce a report. All output is based on user programming of the necessary algebra and selection of the graphing utility. The reports can be viewed, edited, and printed.

It is quite possible for anyone familiar with template creation for a spreadsheet database program to create the equivalent of this program in a relatively short time. While not a user-friendly environment, Edifice operates in a pulldown window format and allows methods and report formats to be saved and recalled depending on the input data type. The environment is very much like that of the early spreadsheets and word processors of the 1970s. Nothing about the operation

is particularly intuitive, and a user community anticipating the MAC or Windows environment would be likely to be disappointed in that sense. Clearly this is a program for a conventional memory PC single-problem, single-user. Attempts to allocate sufficient resources to run Edifice in a Desqview environment were unsuccessful.

Certainly this program will serve to produce reports, and the user willing to work through the setup and testing could have a tool for report writing. The effort would be substantial on the part of the programmer. Perhaps a routine, Register method task manager in a service lab would find it useful.

REFERENCES AND NOTES

- (1) Developed for Mittelhauser Corp. by Peter Jasim, 1991.