$$s(j) = \frac{\sum_{k=0}^{N-1} f(k)\, e^{\frac{-2\pi i}{N} jk}}{\sum_{k=0}^{N-1} g(k)\, e^{\frac{-2\pi i}{N} jk}}$$

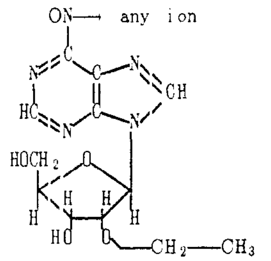

Figure 1. Examples of written complex mathematical expressions and drawn chemical structures within the text. Both examples were written in one line in the text, exactly as shown in the figure.

stored for a later recall under a specific name must be called from the same environment (active keyboard and active key sequence file volume) it was generated in. Suppose we need to write a mathematical formula that we know is already stored as a key sequence file. First, it is necessary to invoke the "mathematical key sequence file" environment from the main menu (shift F9, down arrow, accept, F9, accept, down arrow, accept) and then to switch the keyboard (shift F8, down arrow, accept). After the environment has been set up, the proper key sequence file name has to be typed in while the Ctrl key is held down. Once the mathematical expression (like the one shown at left in Figure 1) is included in the text and shown on the screen, the listed commands have to be repeated in order to bring the user back to its original environment. If further on a structural formula has to be drawn, the environment has to be changed again. We think that it would be much simpler to store the environment attributes together with the key sequence file and to store all files of this kind in one volume or one subdirectory. Such organization would allow, first, all key sequence files to be accessible from any environment, second, the proper environment for the correct execution of the key sequence file to be set up automatically, and, third, the original environment from which the key sequence file was called to be reinstalled immediately after the execution is completed. This will make all handling with the environment unnecessary and transparent to the user, who needs only to select the correct keyboards (shift F8 and select keyboard) for entering simple one-character symbols. For the selection of a proper key sequence file from a number of existing ones, a user-friendly directory display can be organized that would serve the user much better than memorizing the proper names of key sequence files and typing them while holding down the Ctrl key.

What we really like when drawing formulas within the text was the possibility of moving around *parts* of it. This very useful feature enables the insertion of symbols in vertical and horizontal directions into the mathematical expression or chemical formula. As a matter of fact, the entire formula or structure is internally considered as only one line or as a window. The window shrinks and expands automatically (up to a certain size, which is approximately three-fourths of the screen) when symbols, strings, or smaller windows are deleted or inserted. The smaller windows can be shifted around in half-line intervals. By use of this feature, the key sequence files, and different keyboards, an enormous variety of drawings (not necessarily connected with either chemistry of mathematics) can be made within any alphanumeric text.

The manual includes the short reference card, the tutorial, the complete reference manual, and a small template to put around the function keys. The small template is very nice, and we liked it very much until it got lost somewhere in the lab. Afterwards, we had to consult the tutorial every time we wanted to find the meaning of the function keys. The tutorial is clearly written and allows the user to follow the actions accurately. Unfortunately, the method of the tutorial is "follow the leader". We would prefer at the beginning of discussion of each task that there would be a short explanation on the general idea of how the particular task is going to be executed. In addition, an example guiding the user step by step over each single activity should follow. The tutorial describes each task (for example, writing a page of mathematics or a page of chemistry) from the very beginning as if it would be completely different from the other tasks, leaving the user to find out how to use many of the environments in one editing session by switching between different ones. The reference manual is very good in providing almost all answers to questions an experienced user may have. It is quite concise and accurate.

At the time of the review we did not have the HP laser printer, which made the test of high-quality output impossible. (The driver for the Xerox 4045 laser printer, which was at our disposal, was promised before the end of 1988.) We believe that linking the T^3 Scientific Word Processor to the laser printer will show the real value of it. The output will be generated much faster and will make checking the overall appearance of manuscripts much easier compared to checking from the screen or from the slow output via matrix printers.

NMR Simulator and IR Simulator

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Received July 22, 1988

NMR Simulator and IR Simulator are nuclear magnetic resonance and infrared spectrometer simulation programs written by Paul Schatz of the University of Wisconsin and distributed by COMPress (P.O. Box 102, Wentworth, NH 03282). Both programs are designed for IBM PC, XT, AT, or compatible microcomputers, and each supports both CGA and EGA displays, as well as several pen plotters (IBM 7371 and 7372, Hewlett-Packard 7470A and 7475A) and graphics printers (IBM Graphics Printer, Epson FX and MX Series). NMR Simulator requires 256K of user memory and sells for \$95.00, while IR Simulator requires 128K and retails for \$75.00. While no academic discounts are available, both software packages carry a 30-day free examination period. In each case, the program diskettes were supplied in 5.25-in. 360-kB format. No mention is made in the program documentation of the availability of the software on 3.5-in. diskettes. While the diskettes were not copy-protected, the COMPress software license specifies, in effect, that a separate copy of the program must be purchased for each computer on which it is to be used.

Both programs are designed to simulate the operation of a specific spectrometer in such a manner as to allow a person to master the procedures required to record routine spectra. Neither program is designed as a tutorial, however, therefore requiring a user to have significant background knowledge before the programs can be used effectively. NMR Simulator is based on a Varian EM360 60-MHz continuous-wave proton NMR spectrometer, while IR Simulator is based on a Perkin-Elmer 1310 dispersive infrared spectrometer. The programs use the graphics display to depict the instrument controls and chart recorder. Instrument settings are specified through the use of the keyboard or a mouse (Microsoft or Mouse Systems). When a spectrum is recorded, the user sees the spectrum traced in much the same manner as it would be on the actual instrument.

Program Operation. To collect spectra, the user "loads a sample" by specifying a data filename. NMR Simulator provides 3 example spectral data files on the program diskette and 27 additional spectral files on a separate data diskette. Each file contains one digitized spectrum stored in binary format. The spectral files require approximately 12K of disk storage each. The data diskette is organized such that the filenames do not reveal the names of the compounds corresponding to the spectra. A separate ASCII file on the disk provides a correspondence table between filenames and compound names. Four additional data diskettes, each containing 75 spectra, are optionally available and can be purchased for $75.00 each.

The data storage scheme for IR Simulator is idential with that of NMR Simulator. Twenty-eight spectral data files are included on the program diskette, each requiring approximately 2.5K of disk storage. Four optional data diskettes, each containing 75 spectra, can be purchased for $50.00 each.

Once a data file has been loaded, the user is allowed to adjust the instrumental parameters that affect the spectral presentation. Once these parameters have been adjusted, a spectrum can be recorded.

The greatest difference between NMR Simulator and IR Simulator lies in the degree of sophistication of the parameter adjustment section of the programs. IR Simulator allows the user to specify a compressed or full spectral display, to adjust the monochromator to a specific wavelength, to adjust the 100% transmittance line and recorder gain, and to specify a low or higher resolution scan. Unfortunately, in practice, only a few permutations of the parameter settings are encountered. Thus, there is little variety in the operation of the program from one spectrum to the next. NMR Simulator, however, is a very interesting program to use because tremendous flexibility is provided in setting the instrumental parameters. Adjustments for both normal spectral traces and integration traces are included. The user can adjust the R_f power setting, the high-frequency filter setting, the sweep width, and end of sweep position. Spectra can be scanned with the pen up or down, and both coarse and fine spectrum amplitude controls are provided. Before a spectrum is recorded, the user must zero the position of the Me_4Si reference line. The integration controls require the user to adjust a balance control, as well as to set the amplitude for the integration trace. Spectral regions can be expanded and recorded on the same "chart paper" as the full spectrum. Thus, the key practical difference between the two programs is an increased level of sophistication in NMR Simulator that results in each sample requiring different parameter settings and a different operating procedure.

Performance Evaluation. Both programs were tested on an IBM PC-AT equipped with an EGA display and a standard IBM PC equipped with an IBM monochrome monitor and Hercules graphics card. To make the Hercules card compatible with the simulator programs, a resident CGA display emulator program (HGCIBM, Athena Digital, Athens, GA) was used. A Microsoft Mouse (bus version) was attached to the PC-AT to facilitate evaluation of the relative merits of keyboard versus mouse control of the programs. Both programs can be run from diskette or can be installed on a hard disk drive. Even if a hard disk is used, however, the program diskette must be inserted in a diskette drive when either of the simulator programs is loaded. The program documentation specifies that this must be a 360-kB drive, although no problems were observed when a 1.2-MB drive was used.

The two programs were found to perform well. Both simulated the operation of the respective spectrometers with excellent realism. While the layout of the instrument controls suffers somewhat from lack of display resolution, the controls are adequately readable. The programs do not appear to use the increased resolution provided by the EGA display. As with any programs of this type, some time is required to commit to memory the appropriate keys for adjusting the various instrumental parameters. In this regard, mouse operation of the programs is simpler and somewhat more efficient. If a mouse driver is installed, both programs automatically sense the presence of the mouse and allow mouse operation only. The mouse interface to NMR Simulator appears somewhat more forgiving than that of IR Simulator with respect to recognition of the position of the mouse cursor over an instrument control. IR Simulator recognizes only the left mouse button, while NMR Simulator recognizes both left and right buttons.

No problems were encountered in the execution of NMR Simulator. All features provided by the program seemed to work as described. One intermittent problem was observed with IR Simulator, however. The program demands that the recorder gain be checked before a spectral scan is allowed. On occasion, however, the program failed to recognize that the gain had been checked. Several repetitions of this operation were necessary in order for the program to allow a spectrum to be scanned.

Very little difference in program execution speed was observed between the PC and PC-AT. A standard PC with CGA display would thus seem to be the optimum hardware configuration for the programs in terms of economic factors versus program requirements. As a final test, no problems were noted when the simulator programs were executed in the presence of common resident utilities such as Sidekick (Borland International, Inc., Scotts Valley, CA).

Documentation. Both program packages provide a documentation manual describing how to set up and execute the programs. In addition, NMR Simulator provides on-line help screens that summarize its operation. IR Simulator provides no on-line help. The written documentation is adequate, but somewhat terse in its explanations. Several serious typographical errors are present in the NMR Simulator manual, although a correction sheet is included that notes these problems.

Conclusions. In an educational environment, three uses for these programs seem feasible. For non-chemistry majors, they could be used in place of hands-on laboratory training. In this regard, the use of both programs would certainly be better than no laboratory experience. In addition, the programs could be used in teaching spectral interpretation by providing a means for distributing unknown spectra to students. The documentation provides instructions for making separate diskettes containing one or more of the provided spectral data files. Perhaps the best use of the programs, however, lies in training students to use instrumentation efficiently before they enter the laboratory. NMR Simulator could be used particularly effectively in this regard, as it provides a realistic introduction to the use of a proton NMR spectrometer. Given experience with the program, students would be able to enter the laboratory and collect necessary spectra with ease.

In an overall evaluation, IR Simulator would seem much less useful than NMR Simulator. The declining use of dispersive infrared spectrometers makes the program increasingly obsolete. Coupling this with the lack of available permutations of the instrumental parameters makes for a somewhat uninteresting program to use. NMR Simulator, however, is a program that is very topical. It would even seem feasible to use the program in a teaching environment in which a 60-MHz spectrometer other than the Varian EM360 is in use. Instruction in the principles of operation of the EM360 would still be useful to students, even if another instrument is to be used in the laboratory.

For future versions of NMR Simulator, it would be helpful to include two enhancements. First, instrument controls involved in tuning the spectrometer could be implemented. This enhancement would provide students with a more complete experience with the spectrometer. Second, the documentation could be expanded to include more examples. For instance, the use of the R_f power and filter settings could be explored with a demonstrated example.

In summary, NMR Simulator is judged potentially very valuable in an educational setting. With the aid of a mouse, the program is readily used and should prove valuable in teaching students to use an NMR spectrometer. IR Simulator, by comparison, works adequately, but is judged less useful overall.

Microsoft Word, Version 4.0

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Received September 15, 1988

Microsoft Word, Version 4.0, is the latest version of Microsoft's general-purpose word processor for use in the MS-DOS and Apple Macintosh microcomputer environments. I evaluated the MS-DOS version of the program, implementing it on both IBM PC-AT and Leading Edge Model D computers. Both computers were equipped with hard-disk drives and 640 kB of RAM. The software was supplied on six 5-$^1/_4$-in. diskettes, although 3-$^1/_2$-in. program diskettes are available. A minimum of 256 kB of RAM is required for executing Word. Most common displays and display adapters are supported by the program, including all IBM PS/2 displays and adapters. The use of the Microsoft Mouse is also fully supported.

Documentation and Setup. The Word documentation is supplied in three separate volumes: a user's guide, a reference manual, and a printer manual. In addition, plastic keyboard templates are provided that detail the uses for function and keypad keys. Unlike many current software vendors, Microsoft has produced a set of manuals that will withstand much wear and tear. The user's guide is a sturdy D-ring binder, while the other two manuals are produced as equally sturdy spiral-bound books. Overall, the documentation is extremely well organized and lucid. Effective use is made of a two-color format. The index to the user's guide is very complete, making it very easy to refer to individual topics.

Word is configured through the execution of a setup program that is easy to use and foolproof. The user must then select a strategy for learning to use Word to produce documents. A tutorial program, Learning Word, is provided that contains a series of interactive "lessons" that allow a user to step through both basic and advanced editing operations. In my opinion, the experienced computer user will find Learning Word to be annoyingly simplistic in its presentation. The most efficient way to learn to use Word is to type in a short document and then step through the user's guide, chapter by chapter, performing operations as they are described. Through this approach, the entire program can be surveyed in several hours.

Basic Program Operation. Word has two modes: an edit mode, in which text is actively being entered or edited, and a menu mode, in which program or document parameters are set. The <Esc> key or mouse button is used to toggle between modes.

The document being entered is displayed on either a text or graphics screen, depending on the current setting of a function key toggle. This assumes, of course, that a graphics display and display adapter are in use. On the graphics screen, special character formats (e.g., subscripts, superscripts, or italics) appear as they would on the printed document. Scrolling the graphics screen is significantly slower than scrolling the text screen, however. The graphics screen is most useful for performing a quick check on the correctness of entered character formats.

On either screen, a choice of two document displays is provided. The normal display formats paragraphs in such a manner that no lines extend horizontally past the column limit on the display. The actual formating of the document depends on the printer font selected, however. Through a function key toggle, the actual display, termed the "printer display", can be obtained on the screen.

Document editing is performed via a set of basic editing operations initiated by striking either function keys or keys on the numeric keypad. Both sets of keys have four operation levels, accessed as either the key alone or the key in combination with the <Shift>, <Ctrl>, or <Alt> keys. Alternatively, the mouse can be used to perform the same operations. In this regard, the choice between the use of the mouse or the keyboard to control the program is purely one of user preference. Word was written with both types of usage in mind.

A full range of capabilities is provided for moving through the document. Keys are provided for moving to the next sentence, the previous sentence, the next paragraph, the previous paragraph, etc. Deletions are performed by selecting text and then striking the <Del> key. Several keys are provided for selecting text around the current cursor position. The deleted text is normally written to a scratch buffer. Block moves thus involve selecting text, deleting the text to the scratch buffer, moving the cursor to the insertion point for the text, and striking the <Ins> key. This inserts the text currently in the scratch buffer.

Overall, the editing capabilities are complete. My major criticism of this aspect of the program, however, focuses on the requirement for constant movement of the fingers away from the home keys. For example, deletion of the current line is performed by striking <Shift> <F9> <Del>. For such a commonly performed operation, this requires both hands to leave the home keys. For the most common editing operations (e.g., deleting current line, deleting current word, moving cursor to the next word), it would be very useful to have key codes based on the <Ctrl> key and one of the keys within easy