formats. Most commonly used draw-type graphics formats are supported.

• Encapsulated Postscript (EPS). This is a special format for postscript laser printers, which includes paint- and draw-type graphics. You must have such a printer if you use this format.

There are several options on how to place the graphics within your text. You can place it above or below your text or allow text to flow around it in almost any way you can think of. You can enlarge or decrease the size of your image or use the clipping tool to cut out parts of the image. You can even move the image within the clipped frame to find the optimum position.

Steps 2 and 3 can certainly also be interchanged, i.e., place the graphics first and then flow the text around or above it. As an example (see Figure 1) I created a small Wordstar file and placed it in the document using my manuscript style sheet (Times Roman Font). Then I created a line chart using Microsoft Excel. I saved this bar chart in HPGL-Format (i.e., I installed a HP-7475 plotter under Windows and directed the output to a file) and placed it within the document. Finally I created a chemical structure diagram using Beilstein's MOLKICK program. I captured the diagram using the Frieze program of PC-Paintbrush (see above) in VGA resolution and put the respective PCX image into the sample document. Since I captured the screen as a pixel image, the resolution is worse than for the bar chart in HPGL format but still looks pretty good. (Unfortunately, I could not find a chemical drawing program that stores structure images in vectorized HPGL or AutoCad format. Why doesn't someone write such a program?) It took me about an hour to create this sample.

I could not detect any serious flaws in Pagemaker. The program hung twice while I was using it. I am not sure, however, whether it was a problem with MS-Windows-386 or with Pagemaker or with my VGA-Graphics adapter. In both cases I managed to save my work and get back to DOS. I was not able to reproduce the crashes.

Summary. As I mentioned above, Pagemaker is very easy to use, especially once you have set up your style sheets. I use it for preparing overhead transparencies, manuscripts, and even for important letters. Pagemaker does not replace a word processor, and it was never meant to do so. It certainly makes life easier if you need to mix graphics with text or if you need high-quality print output. You should use it with a comparatively fast PC (at least a 12-MHz 80286-type PC) and a high-resolution graphics adapter. In total, Pagemaker can be considered a very helpful tool for the chemist to generate professional-looking documents.

STN Express

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STN Express is a front-end software package produced by STN International to facilitate computer communication and online searching with STN International. The package can be used for automatic logon to other online services (BRS, Dialog, and ESA) as well as for general manual terminal emulation. The package is composed of some well-known computer programs (e.g., Kermit, Plot 10) as well as specially written software (e.g., a chemical formula drawing program).

STN Express is designed to run on IBM/PC, IBM/PC-XT, IBM/PC-AT, PS/2, or 100% compatibles. Our experience with IBM/PC-XT, IBM/PC-AT, Olivetti M24, and AT&T 6300 showed us that there is a difference in the ease of installation as well as speed of use depending on the computer used. Furthermore, the ease of installation depends also on the configuration of the machine used. Minimum requirements are for a 640K RAM with 510K of free memory, one floppy disk drive, and a hard disk with 4 MB of space (2 MB is required for installing the software, another 2 MB is recommended for query building and capture of results), version 3.0 or higher of MS-DOS or PC-DOS. Various options are given for a graphics card (Hercules monochrome or plus; EGA monochrome or color; VGA, AT&T 6300; Olivetti M24; Compaq III; 100% compatibles) and a mouse (Microsoft, 100% Microsoft compatible; Mouse System; IBM PS/2).

The program uses pull-down menus that can be used either with a mouse or with a cursor (and keyboard commands in the case of chemical formula drawing). Using the cursor and the keyboard commands is somewhat slower to begin with, but with time one can do as well as with a mouse.

STN Express enables one (an information specialist or an end-user, an expert or a novice to online searching) to access and search quickly and conveniently the various STN International scientific and technical databases. STN Express provides the user with an automated login to STN International, offline search strategies and chemical structure query formulations, and predefined search strategies as well as special search and display features [scrolling text and graphic, editing command lines, type-ahead (typing while the system is running a search or displaying an answer, the typed material will appear after the next system prompt (=> or :) is displayed)], split text and graphics, and capturing and/or printing an entire (or part) session. For real novice end-users who do not know the STN Messenger command language, STN Express provides the Guided Search module. This module enables everyone to run a simple search (including a chemical structure or a chemical reaction query) with the help of guiding menus. Once the search formulation is completed, STN Express logs on automatically to STN, runs the query, displays the results, and disconnects from STN. The results are automatically captured so that they can be reviewed offline, and if there is a need, the search query can be modified and rerun.

To sum up, STN Express fulfills most of its claims. It enables the user to prepare offline ahead of time his strategy formulation and then upload it after automatically logging into STN. Furthermore, the user can edit and/or reuse one or more of the command lines online or offline. The captured results can be edited either directly (in the case of an ASCII file) or after text and graphics have been split, while the graphics could be added again at a later stage.

The package is accompanied by very good documentation; it is a 332-page manual (an action guide) written very clearly and explaining the various modules of the software in a clear and simple manner. STN International provides good worldwide customer support service for STN Express via its

help desk as well as via its distributed software support group. Unfortunately, this is something that can be said for very few software producers and/or distributors.

The chemical formula drawing feature is one of the best features of STN Express. It is incorporated into the chemical structure query building and into the Guided Search module. It is one of the easiest to use (with a mouse or a curser and keyboard commands) and one of the most friendly chemical structure drawing program I have come upon. Everyone that tried using the drawing program enjoyed it from the first moment, even those for whom it was their first experience in drawing chemical structures using a computer. I myself would like to be able to incorporate the structures created in the structure query formulation in text edited by an ASCII-based word processor.

The package comes with some predefined strategies—15 in the CA File and 17 in the RSWS File. STN is planning to add more predefined strategies in other databases once they are made available by the database producers. As a chemist, I personally do not like too much many of the CA predefined strategies. They seem to be too general—I wonder if forensic and allerg? are valid search terms for a toxicology search; others may think differently. But what is the connection between titrations, titrator(s), titrimetric, etc. and a chromatography search? However, these strategies can be used as they are or after editing and/or modifying by novice or not-so-experienced end-users.

The weak point of the software package is its Guided Search module. The idea behind this module is an excellent one. However, much still needs to be done to this module in order to bring it up to par with the rest of the package.

Some of the limitations of the Guided Search module are the following: The NOT Boolean operator is unavailable; only one proximity operator is available—the W operator, the others (e.g., A, L) are unavailable. In a chemistry search of the CA File the fields Basic, Index, Author, Language, and Type of Publication are searchable. In all other files and in the CA File not in a chemistry search, only two fields are searchable—the Basic Index and the Author fields. There is no reference to any of the standard abbreviations used by CA. All these limitations have quite an influence on the precision recall ratio of the results, or in other words, on the results quality.

These limitations could be overcome by the addition of a chapter to the action guide giving the basics of the STN Messenger command language as well as some basic information about the various databases available.

However, databases that cannot be searched by regular fields (e.g., Basic Index Author) should be removed from the Guided Search module (e.g., BIOCAS and CASOLD, which are available in the Biology and Biotechnology category). Searching full-text databases (e.g., CJACS, CJRSC, CJWILEY) requires a whole range of proximity operators as well as special display formats that are unavailable in the Guided Search module.

There is a need for more online information on the contents of the various databases. (E.g., BIOSIS is one of the databases in the Patent category—how many users know that BIOSIS coverage of patents is limited only to patents granted in the U.S. since January 1, 1986?)

In conclusion, STN Express is an excellent front-end package worth its cost ($595). Its only weak point is its Guided Search module, an excellent idea that needs a good amount of change and/or modification in order to be on a par with the other parts of the package. And, what is more important, it will make searching by the end-user a very easy and simple task.

BOOK REVIEWS

Chemistry by Computer: An Overview of the Applications of Computers in Chemistry. By Stephen Wilson. Plenum Press, New York. 1986. xi + 233 pp. $37.50.

Chemists interested in a highly readable introduction to the basic principles and strategies of computational chemistry will find Stephen Wilson's book very worthwhile. It is particularly directed toward university students (graduate and upper division undergraduate) who may benefit from a general perspective on applications of computers in many familiar as well as unfamiliar topical areas, but it will also be useful to the experimentalist. It provides a focused review of many theoretical principles and equations and illustrates some of the results and consequences of various computational approaches.

While the depth of coverage and choice of examples could be criticized by more specialized readers, it is an important book that, rather than trying to overly "popularize" a new emphasis in chemistry, focuses on several developing topics in chemistry to illustrate the relevance and importance of using the increasingly powerful computer technology that surrounds us.

The book is organized into three parts: I, Basics (34 pages); II, Methods (123 pages); and III, Applications (57 pages). Part I is a whirlwind tour of a range of introductory topics: fundamental properties of isolated and bulk atoms and molecules (Chapter 2), descriptions of CPUs and I/O devices, FORTRAN code for matrix products, and a plea for good software engineering and prospects for parallel computing (Chapter 3).

Part II settles into more in-depth considerations of quantum chemistry, molecular mechanics, chemical kinetics and reactions, and simulations of liquids and solids. In this section are considerations of definitions, equations, computer results and a number of helpful graphics illustrations. Students among the readership should have completed at least a year of physical chemistry.

Chapter 4 (Quantum Mechanics) reminds the reader of the basics of the Schrodinger equation and the matrix Hartree–Fock method, practical aspects of performing a self-consistent-field calculation, electron correlation, and the nuclear Schrodinger equation for diatomics. While ab initio methods are of fundamental importance for small molecules, it would have been helpful for the author to more than just mention the semiempirical methods needed for larger molecule systems (CNDO, MINDO). These programs have become readily available for chemists, and some additional discussion would help bridge the transition to, and help support the need for, the molecular mechanics approach to structure prediction in very large molecules.

Molecular mechanics is covered in considerable depth (Chapter 5), reminding the reader of how little (if at all) this topic is introduced in physical and advanced organic chemistry courses. A nice illustration for the alkanes is presented to give the reader a flavor of what kind of detail is needed for force field parameterization.

Molecular collision theory is surveyed as a prelude to discussions of reaction kinetics in the gas phase (Chapter 6, Chemical Reactions). While equations abound describing the classical mechanical formulation of the problem, the reader is somewhat disappointed with the comment that there "exists a considerable computational technology that treats chemical dynamics using classical mechanics" and is soon referred to "the works cited in the bibliography" for further details of the computational