SpecTool

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SpecTool[1] is a look into the future of computers in chemistry, particularly in chemical education. Many years ago in the BC era (before computers) there were books. When organic and analytical chemists had to interpret unknown structures from various types of spectra, one turned to these invaluable tools. The book by Silverstein and Bassler,[2] now in its fifth edition, is a classic in this field. The authors of SpecTool have also written some good books on this subject area.[3,4]

Today, the need for books of spectral data and interpretation tables are both more needed (as spectral data are being used by more and more chemists) and more difficult to use. The reason for their difficulty is the vast amount of data and correlated data that has become available. That is where SpecTool comes to the rescue. SpecTool is a powerful and easy to use software and database system for interpreting IR, MS, NMR (^{1}H and ^{13}C), and UV spectra which runs on the Apple Macintosh line of computers. (By the end of 1994 there will also be a PC Windows version.) SpecTool is a hypermedia system, which allows for effortless and graceful linking of spectral data. SpecTool consists of over 2000 "tables" or "cards" of spectral data from five different spectroscopies (IR, MS, NMR (^{1}H and ^{13}C), and UV), which one can access and link just by clicking on a mouse button.

The data are divided into these five areas of spectral data, and then within each area the data are grouped by functional group or other structural features. There are many system options. For example, there is a "FIND" module which allows one to search for a term or phrase, like "M-28" (for a mass loss), or "Karplus" (NMR coupling constants), and so forth. Any of the modules are readily accessed from a master "Table of Contents" box which contains a set of buttons (which are really just a "box" full of "cards" of data) for each of the five types of spectra and the three types of information/capabilities available for each one (data, spectra, and tools).

Installation on my Macintosh IIfx in a SpecTool folder was simple and straightforward. The extended version requires about 38 MB of hard disk space. The Macintosh computer should also have at least 4 MB of RAM (and preferably 8 MB of RAM). A good user interface is the difference between delivering or not delivering good technology. While Pacman never needed a user manual, I can only say that SpecTool rarely ever needs a manual, it is so well designed and easy to use. The manual is quite readable and useful, and there is an abundance of examples.

The difference between the "basic" and "extended" versions is that the latter has over 3000 spectra and structures included in the package. Both packages contain lots of reference spectral data and some mass spectrometry utilities (like a molecular formula calculator), as well as a programs for estimating NMR coupling constants, IR stretching frequencies, and UV absorption.

Overall, I think this is an excellent system and should be a requirement for all organic qualitative analysis courses. (I would hope that the distributors of the software will try to arrange special pricing for such university courses, where Macintosh systems are most widespread.) It is also invaluable for researchers doing spectral analysis and interpretation. It gives the user an encyclopedia of data and information, which is made even more valuable by its hypermedia form.

In summary this is a great package that should be on the hard disk of just about every spectroscopist and organic chemist. It is a great example of how computers can be really useful tools for the chemist.

REFERENCES AND NOTES

(1) SpecTool is available from Chemical Concepts, Boschstrasse 12, D-69469 Weinheim, Germany (Phone: +49-6201-606-433. FAX: +49-6201-606-430). The price is DM 1500 (approximately U.S. $950) for a single license and DM 4500 (approximately U.S. $2850) for the extended version. Educational discounts are available. There is a special student price of DM 195 (approximately U.S. $125) for the basic version. A Macintosh version is now available. A PC Microsoft Windows version is scheduled for release by the end of 1994. There is no demo disk available.

(2) Silverstein, R. M.; Bassler, G. C.; Morrill, T. C. *Spectroscopic Identification of Organic Compounds*, 5th ed.; Wiley: New York, 1991.

(3) Clerc, J. T.; Pretsch, E.; Seibl, J. *Structural Analysis of Organic Compounds by Combined Application of Spectroscopic Methods*; Elsevier: Amsterdam, 1981.

(4) Clerc, J. T.; Pretsch, E.; Seibl, J.; Simon, W. *Tables of Spectral Data for Structure Elucidation*, 2nd ed.; Springer-Verlag: Berlin, 1989.

(5) Cadisch, M.; Farkas, M.; Clerc, J. T.; Pretsch, E. SpecTool: A Hypermedia Toolkit for Structure Elucidation. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 286–290.

(6) Cadisch, M.; Pretsch, E. SpecTool: A Knowledge-Based Hypermedia System for Interpreting Molecular Spectra. *J. Anal. Chem.* **1992**, *344* (4–5), 173–177.