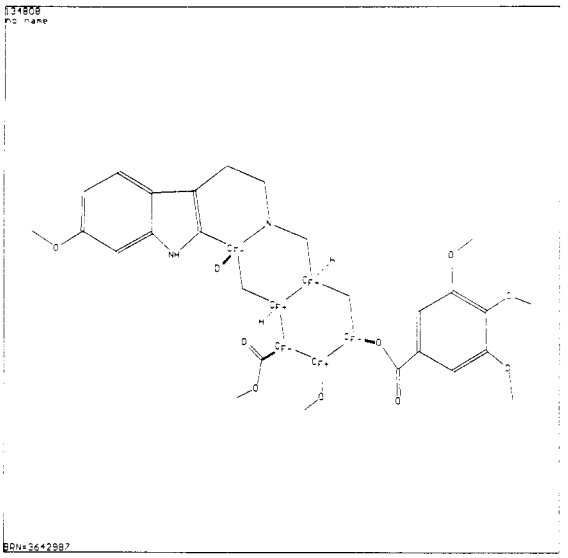

Identification Data - IDE

Beilstein Registry Number	3642987
Lawson Number	12296 289 29358
Chemical Name	<3-2H>reserpine
Molecular Formula	C33H39DN2O9
Molecular Weight	609.69

Preparation - PRE

Starting Mat. (.SB:.SM)	BRN 102014: ent-11,17$b-dimethoxy-18$a-<3,4,5-trimethoxy-benzoyloxy>-15$b-yohimban-16$a-carboxylic acid methyl ester
Reagents (.RGT)	1) TFA, O2, HOAc, 2) CD3OD, D2O, Zn
Other Conditions (.COND)	1) 72h, 2) RT, 2h

Note 1	Multistep reaction

Ref. 1	Awang, D. V. C.; Dawson, B. A.; Girard, M.; Vincent, A.; Ekiel, I., JOCEAH, J.Org.Chem., EN, 55 (14) [1990] 4443-4448

Figure 6. Product from search in which a yohimbane derivative was the starting material.

above), you can choose either structure or data or both, as well as a range of which hits to print out. What is most useful in the display output is the BRN and the Source Field. The former allows you to go online (to STN, DIALOG, or Maxwell/Online—ORBIT) to access the considerable amount of data on a compound which is available online, while the latter allows you to go to the *Beilstein Handbook* to look up additional information on a compound. Thus the online system, *Handbook* and CD-ROM are all well linked and integrated in three useful and complementary products.

The Help menu has five submenus for the areas of help messages. They are **File, Search, Display, Function Keys,** and **Fields Names**. The messages are generally short and clear. For example, Figure 5 shows the help message for the "Identification" search field. In the case of the field names there are three choices to look at. The first has the field names sorted in Field Code order, the second has them sorted in Field Name order, and the third has a hierarchical sort. The last is perhaps the most useful for someone who is new in using the database.

A number of sample searches were performed, and all seemed to provide appropriate results. One sample search for compounds that have an ionization potential between 7-9 electron volts and contain a Br atom and 2 N atoms gave one hit, 1-vinyl-4-bromopyrazole. A second search, for compounds that are synthetized by using a yohimbane derivative as the starting material, gave three hits. One of the resulting three hits is shown in Figure 6.

All in all this is a nice, easy to use, workable system. The developers should be commended for an excellent product, which makes use of the large capacity of the CD-ROM. With CD-ROM drive prices dropping rapidly and some now selling for about $400 (including cables and drivers), I would expect to see more CD-ROM products for chemists come to the marketplace in the near future.[3] The current economics of the pricing of this product are surprisingly reasonable[1] and should make it possible for the Beilstein Institute to get the number of users needed for this product to make it a viable product.

To sum it up I would say that Current Facts is a far more useful chemical information product than a collection of bibliographic citations. This CD-ROM deserves serious consideration for a space on every chemist's computer system.

REFERENCES AND NOTES

(1) Beilstein Current Facts in Chemistry on CD-ROM is available from Springer-Verlag Publishers, 175 Fifth Avenue, New York, NY 10010 (Phone: 212-460-1622; FAX: 212-533-5781). The pricing depends on whether the CD-ROM you buy is for yourself only (individual) or if you are a *Beilstein Handbook* subscriber and if you are in a university or industry/government. The single unit costs for an individual (either in a university or an industrial company) is $490.00 per year. The yearly subscriptions for nonsubscribers to the printed *Beilstein Handbook* are $1490.00 for universities and $2990.00 for industrial companies. For a current *Beilstein Handbook* subscriber at a university (such as a library) the price is $490.00 per year, while the price is $1490.00 per year for a *Handbook* subscriber in industry. The ISSN for this product is 0939-7598. There are also special prices for LAN (local area network) usage for both unviersity and industrial company users. Please contact Springer-Verlag for details on the prices for the LAN version.

(2) DIALOG Information Services, Inc., 3460 Hillview Ave., Palo Alto, CA 94304. (Phone: 800-334-2564 or 415-858-3785; FAX: 415-858-7069).

(3) Heller, S. R. NIST/EPA/MSDC Mass Spectral Database, PC Version 3.0 (1): *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 352-354.

NIST Structures and Properties Database and Estimation Program[1]

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The latest addition to the computerized products of the National Institute of Standards and Technology (NIST) is the NIST Structures and Properties Database and Estimation Program (NIST S&P) written by Stephen Stein, Johannes Rukkers, and Robert Brown of the NIST Chemical Kinetics and Thermodynamics Division. This combination of a database retrieval system and estimation software is designed for both finding and estimating chemical property data. The database contains thermochemical data for almost 4900 compounds or species from three NIST databases. These are the NIST Positive Ion Energetics Database, NIST Chemical Kinetics Database, and the NIST JANAF Thermochemical Tables Database.

The NIST S&P also contains a complete implementation of Benson's group additivity estimation method for gas-phase heats of formation, entropies, and heat capacities. There is

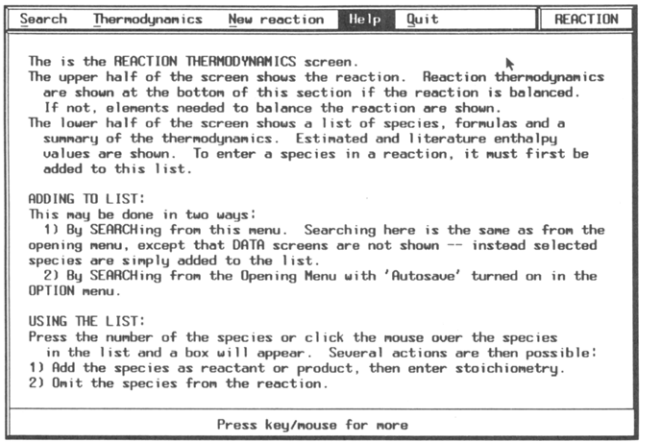

Figure 1. Sample HELP message.

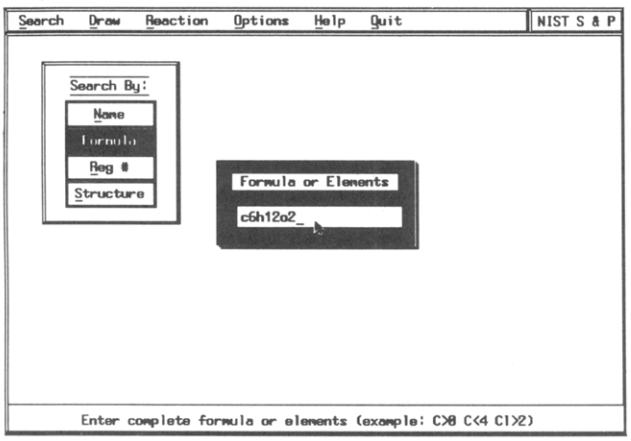

Figure 2. Searching by molecular formula for $C_6H_{12}O_2$.

also a structure-based method for estimating vapor pressures and boiling points. The system estimates properties exclusively from the two dimensional structures drawn, without any need to know about various estimation methods.

The equipment required to use the system is a IBM PC or compatible clone, MS-DOS version 3.1 or higher, with 640K of main memory and a variety of graphics cards from CGA to VGA, work with the system. A color monitor and mouse (for structure entry) are preferable, but not required. The system takes up about 3.2 Mbytes of space on a hard disk. The system is not available for an Apple Macintosh system, and there are no current plans to implement such a version. The entire system came on two high density $5^1/_2$-in. floppy disks. Installation of the system was simple, fast, and easy to perform. I installed the system on both a Compaq 386/25 and AST 486/33 computer with HP laser printers. The automatic loading of the system produces all the files needed to run the system by uncompressing the data from the floppy disk. The 43-page manual is both quite adequate and easy to read, with many examples.

The NIST S&P is organized into five major screen areas or menus. They are as follows: the opening menu, the data menu, the hits menu, the reaction menu, and the drawing menu. There are functions at the bottom of each screen that provide help and other information. The system is searchable in a number of ways, by name, partial or complete formula, CAS Registry Number, and structure or substructure. Help messages abound throughout the system, making it unnecessary to refer back to the manual. There is also on Options module which provides, for example, the option of having the data values either in joules or calories.

The main menu on the opening screen shows the user the three avenues for finding and estimating data in the program.

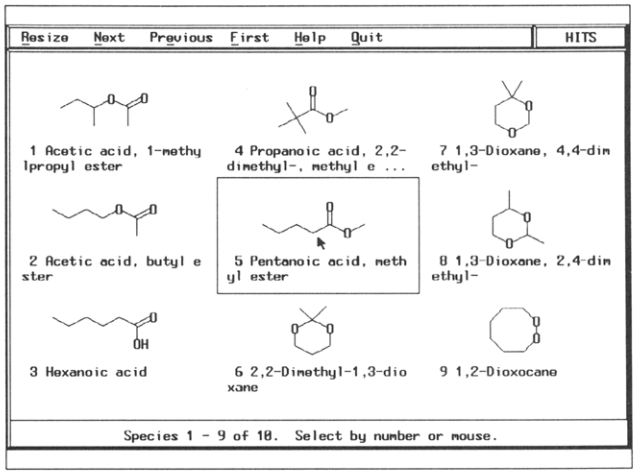

Figure 3. Results from a molecular formula search for $C_6H_{12}O_2$.

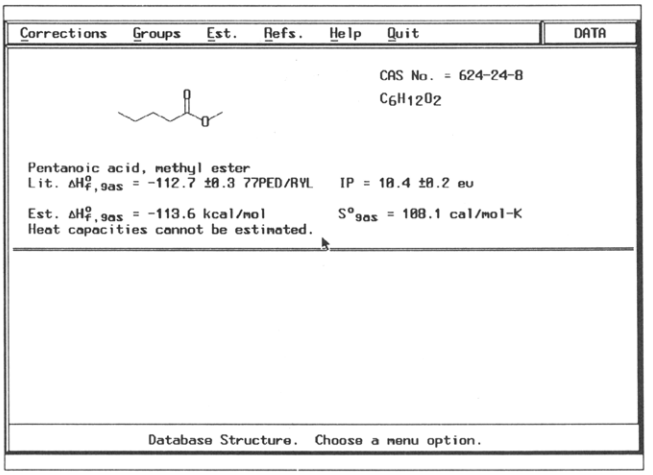

Figure 4. Thermodynamic data for a sample compound.

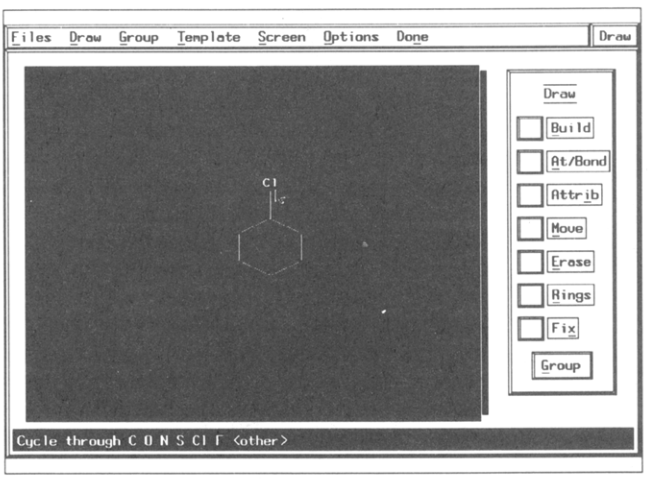

Figure 5. Example of structure drawing, chlorocyclohexane.

They are the Search (find and view), the Draw (structure draw), and the Reaction (compare data and build a reaction).

One can search by name, partial or full formula, CAS Registry Number, or structure. A sample help message is shown in Figure 1, which is then followed by a molecular formula search for $C_6H_{12}O_2$, and the resulting printout, on a laser printer, of the first 9 of the 10 hits is shown in Figure 2. By using the mouse to select the compounds in Figure 2 (the one with the box around it) the literature and estimated data and structure are shown in Figure 4. As one can see from Figure 4, the data is well referenced, an important point which is often forgotten and missing in many database systems.

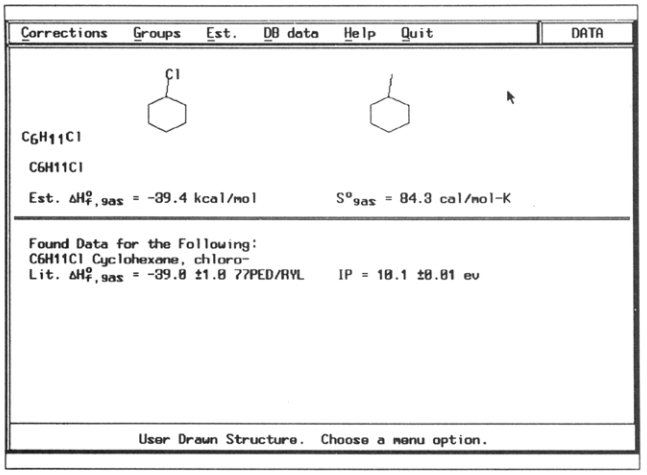

Figure 6. Thermodynamic data for the structure in Figure 5.

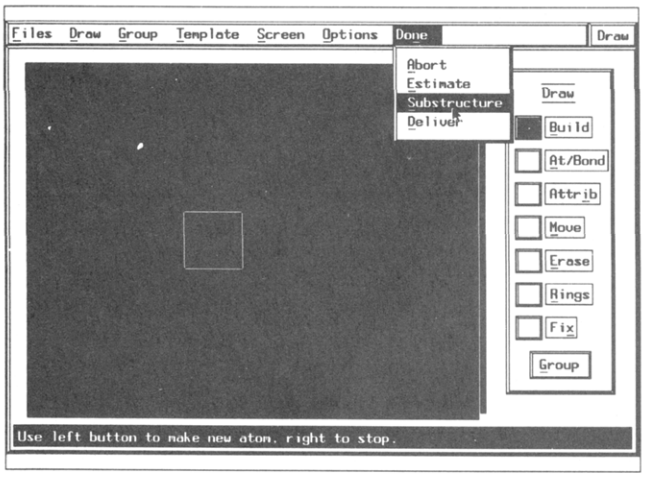

Figure 7. Example of structure drawing for a substructure search.

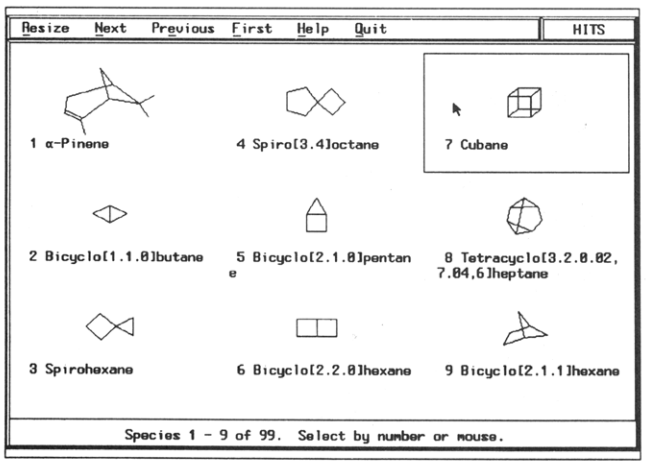

Figure 8. Results of substructure search for four-membered ring compounds.

The structure drawing module was developed at NIST and as such is slightly different from every other independently written structure drawing module. However, since drawing a structure is a rather simple process, learning the few differences for this system should pose no problem to anyone.

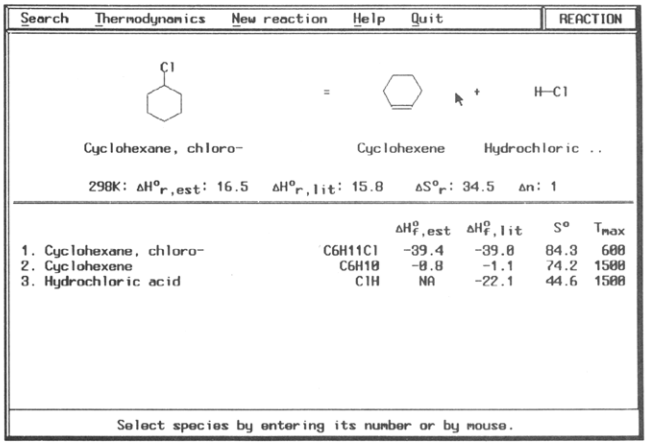

Figure 9. Sample reaction and data estimation.

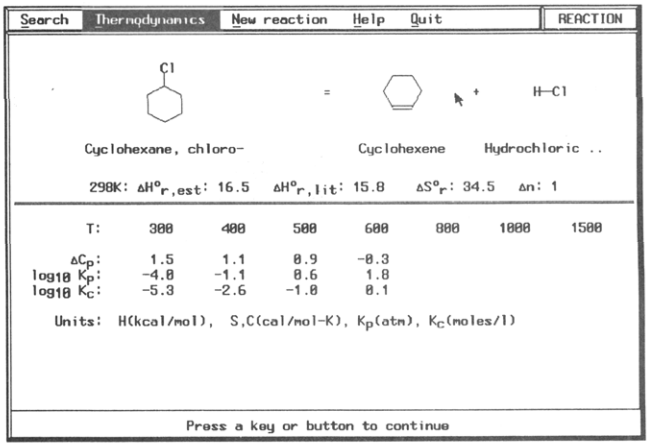

Figure 10. Thermodynamic data for reaction in Figure 9.

Thus no further comments will be about this module, except to show two examples. The first is a structure search for chlorobenzene (Figure 5), and the resulting data from that search are shown in Figure 6. Figure 7 shows a four membered ring which was used to find all structures containing such a ring in the database. Figure 8 shows 9 of the 99 such compounds in the database.

In the Reaction module one can compare data for different compounds and create chemical reactions. In Figure 9 the reaction of HCl and cyclohexene to form chlorocyclohexane is shown, along with the literature and estimated enthalpy of formation for the reaction. Lastly, Figure 10 shows the thermodynamic data (heat capacity and associated K_p, and K_c) over the temperature range of 300–600K.

All in this is a nice, easy to use, workable system. In particular I found the user interface and screen layouts very nice. The developers should be commended for an very nice system product.

REFERENCES AND NOTES

(1) NIST Structures and Properties Database and Estimation Program is available, as NIST Standard Reference Database 25, from the National Institute of Standards and Technology, Office of Standard Reference Data, Building 221, Room A-325, Gaithersburg, Maryland, 20899. The price is $240.00.