CHEMFORM: A System for Drawing Chemical Formulas

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Received July 27, 1994

CHEMFORM is a collection of bit-map image files designed to be used in conjunction with Paintbrush[1] in Microsoft Windows[2] 3.0 or 3.1 to produce two-dimensional chemical formulas.

The library consists of 167 bit-map imagefiles that are pasted into the Paintbrush drawing area, as required. The substructures, bonds letters, and other symbols present in the files can be moved, copied, joined, cut-out, or flipped, using the Paintbrush's functions to produce the desired structure.

CHEMFORM is not a program in itself, but it is actually a collection of images; therefore a strategy aimed to the generation of the formulas is required prior to commencing the actual pasting or deletion of fragments. The design of a strategy is more important in this case than in fully integrated packages for the same purpose, since the program lacks of any chemical understanding.

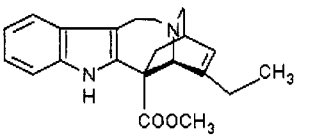
In most cases, the first step in producing a formula requires building some skeleton for it. There are three ways in which the basic moieties can be constructed using CHEMFORM. First, structural elements from the library could be joined together, second, the structure can be created from scratch using solely bonds that are present in one of the files, or third, a substructure in the library can be broken down into smaller subunits that conform to the basic skeleton. Then, side chains and other substituents can be added utilizing the same or additional imagefiles. In general, building a new structure requires a combination of all three strategies.

The number of elements that compose the CHEMFORM library is relatively small; however, no obvious limits exist to the types of formula that can be represented. The implementation in Paintbrush allows the immediate generation of other elements that may be required to build a formula but are not explicitly present in the bit-map files.

CHEMFORM is extremely simple to use and comes with detailed instructions. The manual is divided in two parts: a user's manual and a formula book. The first explains the use of the program in a step by step manner and with numerous exercises. This manual is well written and very friendly. The second is a formula book with over 50 examples with a schematic description of the strategy used to build the molecule. The examples take anywhere from a few minutes to close to 2 h, and it shows a spectrum of fairly simple to quite complex structures.

Since all operations are carried out by Paintbrush, some degree of familiarity with this program is required. For the most part, explanations for the most commonly used Paintbrush commands are provided with the CHEMFORM documentation. The CHEMFORM user manual provides brief descriptions of the most commonly used options, including cutting, moving, pasting, resizing, and flipping horizontally or vertically.

A positive aspect of CHEMFORM is that its implementation using Paintbrush facilitates the communication with other programs. The BMP or PCX files generated can be readily important into many word processing and some desktop publishing programs. The use of Paintbrush can also be advantageous to enhance the quality of the presentation, in a creative manner.



Catharanthine

Figure 1. Structure for catharanthine generated using CHEMFORM. 300% scaling at printer resolution and a laser printer were utilized.

Despite its simplicity, the system is more laborious and takes on average longer to build a formula with it than what it would take with other fully integrated programs for this purpose. One of the least attractive aspects of the system is the difficulty to locate the most convenient fragment to build a new formula throughout the library. A general directory of the structures in the different files is only provided as an appendix to the user manual, which to some extent facilitates the task.

In addition, the system has some idiosyncrasies that are due to the use of bit-map images. For instance, since this is not a program in itself, the system is unable to correct built-in asymmetries in the images when building fused rings. Thus, depending on whether the rings are fused through a bond represented diagonally or vertically different types of fragments have to be added. There is a work-around the problem which can be fixed using the Zoom-In command and correcting each pixel individually. Indeed, in many other instances the use of the Zoom-in command results also in a significant improvement in the appearance of some formulas.

Also due to the use of bit-map images, the lines that are in orientations other than horizontal or vertical have jagged outlines that appear when the figures are printed at a normal resolution. The way around this problem is to reduce the size of the images and figures until the jagged outlines appear less obvious. However, this may not be always practical. A sample of the quality of the output is presented in Figure 1. The jagged lines can be noted even at this relatively small size.

The formula can be printed at different scales, using Paintbrush. Most figures are reproduced best if two or three times the printer resolution is chosen. In the event that a fractional enlargement is required, then this should be done reprographically, because otherwise the results are not as satisfactory. The use of laser printer is recommended, but ink-jet printers produce very good results, and even dot-matrix printers can generate an acceptable figure.

CHEMFORM can be obtained by contacting F.O. Corner 11, The Orchard, North Holmwood, Surrey, RH5 4JT, U.K. Also a shareware version can be obtained from the Public Domain & Shareware Library, Winscombe House, Beacon Rd., Crowborough, Sussex, TN6 1UL. The shareware version does not contain the formula book and costs approximately £ 6. The minimum hardware requirements to run CHEMFORM are a 286 PC and 614 Ram.

REFERENCES AND NOTES

(1) Microsoft Windows Paintbrush is a trade mark registered by Microsoft Corp.
(2) Windows is a trademark registered by Microsoft Corp.