ConSystant and Chemeleon

Venkat K. Raman

Chemical Abstracts Service, Columbus, Ohio 43221

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The use of several different pieces of PC softwares by chemists often presents a problem when an attempt is made to exchange data between the various software packages. Most of the chemists use their own data formats and hence have limited, if any, ability to load their data onto softwares supplied by other vendors. Unfortunately, most of the vendor-supplied programs used by chemists for drawing chemical structures, modeling them, databasing them, etc., have their own file formats.

To solve this problem, ExoGraphics has introduced a new product called ConSystant, which is a utility program to be run on IBM PCs. With ConSystant, one can interconvert data from several chemical data formats, including MOL (of Molecular Design), SKC (of ISIS), HyperChem HIN (of Autodesk), MPG (of HawkScientific), Strings (of SMILES), etc. This utility will definitely facilitate the exchange of data between many of the most popular chemical software packages available on the market today. A directory full of files can be interconverted with ConSystant. Many of the chemists use software packages which are designed for the Microsoft Windows environment. It is extremely convenient to "cut and paste" data between chemical application with Windows. ConSystant includes an unique utility called Chemeleon, which lets the chemist cut and paste. Under Windows, the clipboard is monitored by the loaded Chemeleon for recognizable chemical data. When the data are located, Chemeleon automatically and transparently converts the data to the desired format of whichever application is running.

INSTALLATION

Both ConSystant and Chemeleon are written on diskettes which are supplied with the package. The disks are of common PC sizes (3.5 in. and 5.25 in.), and the software should be installed onto a hard disk before it is used. An INSTALL program is on the disk which executes the installation process. After installing the master disks in an appropriate disk drive (need not necessarily be drive A), the files are uncompressed from the master disk to the directory specified on the user's hard disk. There are two main program files: CS.EXE (ConSystant) and CHEMEL.EXE (Chemeleon). If the presence of Windows is detected during the installation, the user is asked if the Windows configuration should be adjusted to have the Chemeleon loaded automatically. With the selection of this option, the only Windows file modified is the WIN.INI file; the existing WIN.INI file is saved as WIN.OLD. CS.EXE is a dual-mode DOS/Windows executable file.

SOFTWARE SETUP PROCEDURE

In a DOS environment, typing CS at the prompt starts operating the software. Under Windows, three successive steps are to be taken. These include adding ConSystant to a program group, adding Chemeleon to a program group, and loading Chemeleon automatically in Windows. The source format is the format that the user is converting from, and the Destination format is the target format.

USE PROCEDURES

ConSystant converts a file (or files) in a single directory from one format to another using a single command. Standard DOS "wildcard" characters (* and ?) are supported. As it converts a file, a log file (CS.LOG) is generated in the same directory; this temporary file is destroyed and recreated each time a conversion is made. The output file keeps the same root as the original and modifies the extension. The default extensions include .ALC, .CDT, .SKC, etc. An option exists for specifying the directory where the output file would reside. While the information required by ConSystant is the same regardless of whether the program is executed from DOS or from Windows, the different interfaces accept the information differently.

The ConSystant–DOS Interface. When started at a DOS prompt, an initial screen appears which has three sections—a title block, a status display, and a menu block. Commands are entered by selecting them from the menu block (File, Input, Output, Config, etc.). At the start, the appropriate input and output formats are set up. To select a format, the highlight bar is moved using the arrow keys. The "File" command is used to enter the file name mask of the file(s) to be converted. Every time ConSystant performs a file conversion, it "remembers" the current directoy and saves it for the next time ConSystant is used. The "Options" command enables one to access commands for setting user-defined options.

The ConSystant–Windows Interface. The commands are entered via the pull-down menus, when ConSystant is started from within Windows. There is a "Clipboard Conversion" command which allows a conversion to proceed in the Windows clipboard. After the input and output formats are selected, the "Convert" command is used to produce a dialog box into which the user enters the file name mask of the file(s) to be converted. Conversion begins after clicking on the "OK" button. ConSystant is controlled both via the command line and via dynamic data exchange. The command (WM_DDE_INITIATE) begins a "conversion" with ConSystant. WM_DDE_EXECUTE is the command for controlling ConSystant.

Using Chemeleon. This Windows-based program automatically converts chemical data which may be in the Windows clipboard to a different chemical formula appropriate to the active program. Chemeleon is automatically loaded when Windows starts. It comes with many predefined programs. If it is desired that Chemeleon be stopped temporarily, then "Pause" in the "Start/Stop" menu is chosen. Chemeleon is unloaded by choosing "Exit" from the "File" menu.

ConSystant and Chemeleon are used for interconverting many different chemical format files. Connection tables, which are formats with lists of atoms and bonds, are given. Others are linear notations, where the molecule is described as a continuous stream of atom and bond data. ConSystant can also convert chemical data to simple graphical output.

LIMITATIONS

There are certain generic limitations which apply to all of the chemical data formats handled by ConSystant and Chemeleon. There is a general limit of approximately 600 bonds and 600 atoms in the file to be converted. All atoms from 1 to 103, in the periodic table, are recognized. ConSystant attempts to detect rings and determine if they are aromatic. Some file formats have the ability to store molecules which contain disconnections, or store multiple molecules within a single file.