NMR NOTES #4

PC-Based NMR Processing Software

There are several programs available for processing and manipulating data from the Varian NMR spectrometer systems using IBM-PC clone computers. Both the Varian spectrometers and the PC clones use a 5-1/4" floppy disk drive, which provides an easy mechanism for moving spectral data between the instrument and the PC. Unfortunately, the instrument does not write a DOS compatible disk, but the disk is compatible with the PC hardware, and we have developed a software package that will read the Varian disks and convert the data into a form that is usable by several of these different processing programs. The conversion utilities are very simple and will run on virtually any PC clone computer, and do not require any special hardware capabilities. The various NMR processing packages on the other hand often do have specific requirements. This is a summary of the packages available and the known requirements.

PCNMR+ - This is a very nice menu driven program from the University of Wisconsin that does a good job processing spectra. It will run on '286/'386/'486 machines with 640k memory with no problem. A math coprocessor is recommended but not required. It does require EGA graphics and a 3-button mouse. Standard output is to HPGL pen plotters, and the current version has the capability of writing output to a disk file instead of only a hardware port. making it possible to capture the HPGL file to include in a word processing document. There is also provision for plotting spectra to a ProPrinter dot matrix printer, but this not a very satisfactory alternative. I have a program called PrintGL which will print an HPGL file to a variety of different printers including laserjets. This provides a very good quality output on 8-1/2 by 11 inch pages. A newer version, PCNMR For Windows, is available. I have not yet looked at it to see what the differences are, although it will not currently read the lybrics file format written by our conversion software.

NUTS-32 - This is an application that runs under Windows 3.1/Windows NT/Windows 95 and is capable of processing both 1D and 2D NMR data as well as arrayed data. It is still under active development, so that new capabilities are added on a regular basis. This package can read data files converted from the Gemini/XL/VXR spectrometers, imported either by floppy disks or LimNet, and can directly import UNIX format files generated by the Unity and UnityPlus consoles. Since this is a Windows application, the resources available to the program depend on the devices and drivers accessible to Windows. The program itself is very math-intensive and requires a fast '386 or '486 machine (with math coprocessor) to give reasonable performance. It will not run on a '286. Operation under Windows 3.1 requires the installation of the Win32s 32 bit extension package.

Another option for using a PC (or MacIntosh) to process NMR data is to use the PC as an X-terminal in order to run the VnmrX program on the Sun Workstation. This requires installing an ethernet card to get onto the network (NOT a serial COM port connection), and installing the X-terminal emulator software. X-One from Grafpoint has a very nice emulator with the required TCP/IP transport built in. XWIN32 is available under a campus site-license. This emulator is a 32 bit application that will run under Windows 95/Windows NT, or Windows 3.1 with the win32S 32 bit extensions installed. As a Windows application, it uses the TCP/IP stack defined for Windows. This can be the native stack in Windows 95, the Trumpet Winsock, or a stack from a separate networking package. Any emulator will require several Meg of additional memory, and you will want the fastest, highest resolution video card that you can get for adequate performance. A display of at least 1024 by 768 is required for reasonable performance with the VnmrX software. This configuration will permit you to run the Sun workstation remotely, plot and print using the hardware devices connected to the Sun network, and possibly plot to devices interfaced to you local PC.