

Introduction to the UNIX Operating System and Open Windows Desktop Environment

Welcome to the Unix world! And welcome to the Unity300. As you may have already noticed, there are three Sun Microsystems workstations (“Suns”) in the room housing our Varian 300 MHz spectrometer. One of them (**unity300**) is used to control the instrument and the other two (**ernst** and **bloch**) are used for data processing only. These workstations and the software were upgraded in 2002 so that we have an Ultra-10 with LCD monitor for unity300, and two SunBlade 100 workstations for **ernst** and **bloch**, all using VNMR version 6.1C.

Although it is possible to treat the computers as black boxes that run the instrument and process your data, we prefer to have you learn at least some basics of the Unix environment and data management in that environment. This will save you time and help avoid headaches later on. The Unix operating system is similar to DOS, if you are old enough to remember the pre-windows operating system for PCs. The main difference between Unix and the operating systems used for the personal computers is its ability to provide a multi-user environment, where several users can use the same workstation at the same time without interfering with each other.

Unix is designed to provide a multi-user environment. Each user has his/her own “territory” within the computer, under the heading of the “home directory”. A complex system of “permissions” makes sure that no one else can mess with your data. Initially, people were using Unix computers by logging in remotely via very slow phone lines. As a result, all of the essential Unix commands are very short and consist of two or three letters so that you don’t have to spend time entering a long command and then re-entering it because you misspelled it. For the same reason, Unix is case sensitive (cp and Cp are two different commands!). This can cause serious problems if you accidentally hit the “Caps Lock” key on your keyboard.

1. Logging in.

Logging in is simple as long as you know your login name and password (both are case sensitive). There is no difference which workstation you log into, except for one thing: you can only acquire NMR data from the unity300.

Click on: Options / Session / Open Windows Desktop

Please Enter Your User Name: smith <Enter>

Please Enter Your Password: password <Enter>

After your name and password are validated, the whole screen will get covered with a blue varian logo and a mouse pointer will appear. This is called the Open Windows Desktop Environment. It’s similar to the Microsoft Windows desktop, with a bunch of independent windows operating the software. The windows will appear one by one until you have the whole VNMR screen in front of you.

2. Logging Out: The System Menu.

Point with the mouse at the background (“wallpaper”), press and hold the right mouse button. A System Menu will appear with several options:

```
Workspace
Acquisition Status
VNMR Online
VnmrX
Programs >
Utilities >
Properties . . .
Help . . .
Desktop Intro . . .
Exit . . .
```

Selecting **Exit** will, if confirmed, exit the Open Windows desktop and automatically log you out. To select the option simply highlight it and release the mouse button. You will be prompted to confirm:

Please Confirm Exit from Window System: [Exit] [Cancel]

Click on **Exit** to log out. **NOTE:** Be sure to exit the VNMR software before logging out! Enter “exit” in the text entry window of VNMR. Failure to properly exit VNMR will cause problems for you the next time you log in to **unity300**, **ernst** or **bloch**.

3. The Unix Shell

Console Window. There are two Unix shell icons on the desktop. The console icon is in the upper right hand corner of the monitor screen, hidden behind the Acquisition Status window. You can open this window by moving the Acquisition Status window aside (click on the top bar of the window, hold down the mouse button, and “drag” the window to the left) and clicking on the small square icon labeled “console”. This will open into a window with a text prompt. You can enter any Unix commands at the text prompt, and use this window to check files, delete files, move files, etc. To close the window (reduce it to a small icon again), click on the top bar with the right mouse button and drag down in the pull-down menu to the “close” selection. **DO NOT EXIT** the window, just select **close** to reduce it to an icon.

VNMR Window. The other Unix shell is the **VNMR window**, which appears as another small square icon labeled VNMR, below the Acquisition Status window on the right side of the screen. This shell is the one which ran the VNMR software, so as long as VNMR is running this Unix shell is “tied up”. When you type exit at the VNMR text entry window, the program is closed and the VNMR shell is available again. Click on the icon

to open the window, and you will see the command “Bye” at the Unix prompt – this is the exit command from VNMR. To re-start VNMR, simply hit **Enter** to get the Unix prompt and enter **Vn** to start the software again. As with the console window, you can minimize it to an icon again by clicking on the top bar of the window with the right mouse button and dragging down to the **close** option. Again, you never want to **exit** this window.

4. Useful Unix Commands

After you have acquired and saved your data you will want, at some point, to delete, copy, or move data from one directory to another.

Unix files are organized into tree-structured directories (or folders), similar to DOS in most ways. You use **cd** to change directories, “.” to denote the current directory, and “..” to denote one directory above the current directory in the tree (the “parent” directory). One maddening difference: Unix uses a “/” (slash) where DOS uses a “\” (backslash). Keep in mind that this is a multi-user machine and you can wander out of your disk area. For example, “/” denotes the root (top) directory for the entire computer, not just for your account. If you get lost, enter **pwd** to find out where you are, and **cd** alone to get back to your main (“home”) directory. In the list below, note that commands and the filenames are always separated by a space.

ls	list files and subdirectories;
ls -l	same as ls but gives details on each file
more filename	view a text file, scrolling one page at a time;
cat filename	spits out a text file to the screen all at once
without	scrolling;
rm filename	remove a file;
cp file1 file2	copy file1 to a new file called file2;
mv oldname newname	renames a file, also will move a file if the new name specifies a different directory;
pwd	shows the name of the current directory;
cd directory	changes directories;
mkdir directory	creates a directory;
rmdir directory	deletes a directory;

Note that in the above commands *filename* can be a simple filename, a path relative to the current directory, or an absolute path starting with the root directory:

filename	A file in the current directory
dir1/dir2/filename	relative path under the current directory
/dir3/dir4/filename	absolute path under the root (/) directory

Also in the above commands *directory* can be a simple directory, a path relative to the current directory, or an absolute path:

<i>directory</i>	A directory immediately under the current directory
<i>dir1/dir2</i>	A directory in a path relative to the current directory
<i>/dir3/dir4</i>	A directory in an absolute path under the root (/) directory

Your “home” directory is */export/home/group/login*, where *group* is your research group (hruby, hall, bates, etc.) and *login* is your login name (jones, smith, etc.). You will end up in this directory every time you log in or enter **cd** alone. You can save you data files here – NMR data will go into the directory **vnmrsys/data** under your login directory.

5. Archiving NMR Data

Why archive? Because someday you will want to publish your data or interpret it again in the light of new results, and the paper plots you made will not be adequate. Trying to measure J-coupling values with a ruler is a thing of the distant past! The easiest way to archive your NMR data is to copy it to a PC using the ftp (file transfer protocol) program, and then “burn” the data onto a CD-ROM using a CD writer. The Computer Graphics Facility has a PC with a CD burner, and there is also a Linux PC in the Bruker AM-250 room with a CD burner.

6. Using the *vi* Text Editor

The **vi** (pronounced vee-eye) editor is used to create new text files and change existing ones. It is quite a powerful interactive, visually oriented editor, although **vi** is not a text formatting program. It does not justify margins or provide the features of a word processing system. Everyone loves to hate **vi**, but it is the most basic way of modifying a text file, especially when using a Unix computer remotely over a network.

vi has two modes of operation, the *Command Mode* and the *Insert Mode*. While in the command mode, **vi** accepts keystrokes as commands, responding to each command as you enter it. In the insert mode, **vi** accepts keystrokes as text, displaying the text as you enter it.

At the beginning of an editing session, **vi** is in the Command Mode. There are two commands that put **vi** in the Insert Mode: “insert” (**i**) and “append” (**a**). Note that all **vi** commands take effect immediately; you DO NOT have to press <Enter> to indicate the end of the command. Also keep in mind that **vi** is case sensitive: **I** and **i** DO NOT represent the same command! When you press the <Escape> key, **vi** always returns to the Command Mode. Unfortunately, **vi** does not indicate in any way the mode it is currently in. If you are not sure what is going on, just press the <Escape> key and you will end up in the Command Mode.

Calling vi. Enter **vi filename** in a Unix shell to start editing a file. The screen should clear and the text of your file should appear on the screen. If the file does not exist, an empty file will be created. When the end of the file is displayed on the screen, **vi** marks lines that would appear past the end of the file with a tilde (~) at the left of the

screen. Every line on the screen, except for line 1, is marked with these symbols when you start editing a new file.

The Quit command. Should you want to exit **vi** without saving the changes you made, enter **:** (colon) which will move the cursor to the bottom line of the screen, and then enter **q!** followed by <Enter>.

The Exit and Save command. If you want to exit and save your work, enter **ZZ**.

Entering text. Once you have gained access to **vi**, put **vi** in the Insert Mode. Now you can start entering text, pressing <Enter> key to end each line. Note that **vi** WILL NOT “wrap” (automatically return to the left margin) long lines for you! Press <Escape> when you are finished.

Moving the cursor. While **vi** is in the Command Mode, you can position the cursor over any character on the screen using the four commands **j** (up one line), **k** (down one line), **l** (right one character) and **h** (left one character). Note that these four keys are right under or next to the fingers of your right hand on the keyboard (**j k l ;**). You can go to a specific line number by entering the number follow by upper case **G**. Upper case **G** alone will take you to the end of the file.

The Insert Command. The **i** command puts **vi** in the Insert Mode and places the text you enter *before* the character indicated by the cursor.

The Append Command. The **a** command is similar to the **i** command, except that it places the text you enter *after* the character indicated by the cursor. The **A** command places the text after the last character on the current line.

The Open command. The **o** command opens up a blank line below the line indicated by the cursor, places the cursor at the beginning of the new line, and puts **vi** in the Insert Mode. The **O** command does the same thing *above* the current line.

The Join Command. The Join command, **J**, joins two lines of text. It joins the line below the current line to the end of the current line. It inserts a space between what was previously two lines and leaves the cursor on this space.

The Delete Character command. The **x** command deletes the current character.

The Delete Line command. The **dd** command deletes the current line. To delete the next 10 lines, starting at the current line, enter **10dd**.