# 5. AM/AC Spectrometer Software

by *cg fry*: created 12/10/94 – updated 20.Aug.2002

## I. ADAKOS (Aspect Disk And Keyboard Operating System)

- ADAKOS is the base operating system of the ASPECT computer, the acquisition and analysis computer on the AM spectrometers. Some functions of ADAKOS include listing of directories, batch copying or deletion of files, renaming of files, initialization of new disks and restoration of deleted files. This program is started automatically whenever the computer is rebooted (**<STOP><CLEAR><DISK>**).

  All ADAKOS commands have two or three letters, e.g., **DIR**, **COP**, and **DEL**.

  **MO** (monitor) to exit to the ADAKOS subprogram from DISNMR.

  *** DSP ON** ("*" is the AM-console prompt) to turn on the display.

  **DIR** to list all files in the directory: **H** to halt and **C** to continue. **<ctrl> Q** to stop.

  **SDIR **.*** for sorted directory (sorted by alphabet; can be quite slow).

- A filename has up to eight characters, followed by up to four characters. The wild card * represents only groups of four characters for *only* blocks 1-4, 5-8 or for the suffix. **DIR *.*** will only show filenames having four characters or less. **DIR aa*.*** is invalid, since * cannot represent the 3rd through 6th characters. ? can be used for any single character (only available in ADAKOS, unfortunately not in DISR).

- D1 is the system disk. Use F1 for the floppy disk. The disk designation must follow the filename unless it is the default drive (D1). e.g.,

| | |
|---|---|
| **DIR **.*=F1** | to list all files on the floppy. |
| **COP <input file>/<output file>=F1** | to copy a file from disk onto a floppy. |
| **COP <input file>/=D2** | to copy with the same filename. |
| **COP **.*=F1/=D1** | to copy every file on a floppy to the hard disk. |
| **DEL <filename>=D1** | to delete a file from disk. |
| **DISR91** | to run DISNMR (**RUN DISNMR** on WP-console). |

## II. DISNMR

### *A. Control Keys and System Commands*

| | |
|---|---|
| **<ctrl> D** | toggles the grid ON and OFF on the display; |
| **<ctrl> L** | toggles between the lock display only, the data only, and both. |
| **<ctrl> H** | halts following next acquisition; active only in current job |
| **<ctrl> E** | halts immediately; does not save data; active only in currect job |
| **<ctrl> K** | halts all activity including acquisitions, plotting and printing; active in all jobs; use only as a ***last resort*** (try <ctrl>H first, the <ctrl>E) |
| **<ctrl> X** | toggles between 1st and 2nd sessions |
| **<ctrl> Y** | toggles display from interleaved to separate quadtrature channels |

- **OUT <ret>** for setting up output devices.
  COMMAND INTERPRETER? **B** (both).
  OUTPUT DEVICE? **P** (printer only).

### *B. Files in DISNMR*

- In DISNMR, any file except the current one can be deleted in the same manner as above. **DIR** is also available, but the wild character **?** can't be used. The * wildcard can only represent characters 1-4 or 5-8, or the suffix:

| | |
|---|---|
| **DI *.*** | will list all files having 4 characters or less in prefix |
| **DI **.*** | will list all files |
| **DI cgf1*.*** | will list all files starting with **cgf1** |
| **DI cgf*.*** | *not allowed* since * must start in position 1 or 5 of prefix |
| **DI cgf?*.*** | *not allowed* in DISNMR; ok in Adakos |

- There are many types of files:

| File Type / Process | 1D data files | 2D data files | Job files | Shim files | Automation |
|---|---|---|---|---|---|
| Common suffix | **.001 | **.SER | **.1DJ<br>**.2DJ | **.SHIM | **.AU |
| Disk I/O | WR, RE | (.AU writes), RE | WJ, RJ, PJ | WSH, RSH | EDIT, AU |
| Directory | DI:F (FIDs)<br>DI:S (spectra) | DI **.SER<br>DI **.SMX | DI:J | DI:Z | DI:A |

- **TI** will allow entry of up to 80 freeform characters, stored with data file. *Users should include a brief sample description, and notebook number and page in the TI area.*
- **RE <filename>** to read a file ("**?**" following any command opens a helpfile). One can also save or read files from an external 8" or 3-1/2" floppy disk (F1) as follows:

  **WR <filename>=F1** to save a file to floppy
  **RE <filename>=F1** to read a file.

- **COP** and **DEL** commands work as in Adakos.

### *C. Common Acquisition Commands (WJ, RJ)*

**AQ** – acquisition time
**AS** – automation setup
**CO** – continue acquisition
**CPD** – composite pulse decoupling (Waltz-16 decoupling)
**DO** – decoupler gated off
**DE** – pre-scan delay
**DP** – decoupler power (actually, decoupler attenuation in dB)
**DS** – # dummy scans
**GO** – begin acquisition
**GS** – GO setup mode
**HD** – pulsed homonuclear single frequency decoupling
**II** – initialize interface
**NE** – # experiments
**NS** – # scans
**O1** – transmitter offset frequency
**O2** – decoupler offset frequency
**PO** – decoupler power off
**RD** – relaxation delay
**RG** – receiver gain (actually, receiver attenuation in dB)
**RGA** – automatic receiver gain setting
**SF** – spectrometer frequency
**SI** – spectrum size
**SW** – sweep width
**TD** – time domain size
**ZE** – zero data and initialize for acquisition

### *D. Common Pulse Sequence Commands and Parameters (WJ, RJ)*

**( ):D** – ( ) operates on decoupler
**An** – transmitter quadrature phase
**Bn** – decoupler quadrature phase
**Dn** – delay length for nth delay
D0 is 2D $t_2$ delay incremented by IN (*not* the loop parameter)
**FL** – input frequency list
**GO=j** – perform GO, jump to line j when finished; continues NS times
**IF** – increment file number
**IN=j** – loop index jumps to line j; continues NE times
**IN** – time incr. in 2D set by SW1
**O2** – read decoupler frequency, increment list pointer
**Pn** – pulse length for nth pulse
**Sn** – decoupler power setting

### *E. Common Data Processing Commands (WJ, PJ)*

**AI** – absolute intensity
= 0 (default) autoscales
= 1 absolute intensity
**AT** – additive transfer of two spectra
**BC** – apply linear baseline correction
**FT** – Fourier transform
**PK** – apply phase correction last stored in **EP** mode
**SR** – spectrum reference frequency
**EM** – exponential multiply

$$E_i = \exp\left[-\pi t_i \cdot LB\right]$$

chose **LB** ~ linewidth
**GM** – gaussian multiply

$$G_i = \exp[\ -\pi \cdot t_i \cdot LB + \frac{\pi \cdot t_i^2 \cdot LB}{2AQ \cdot GB}\ ]$$

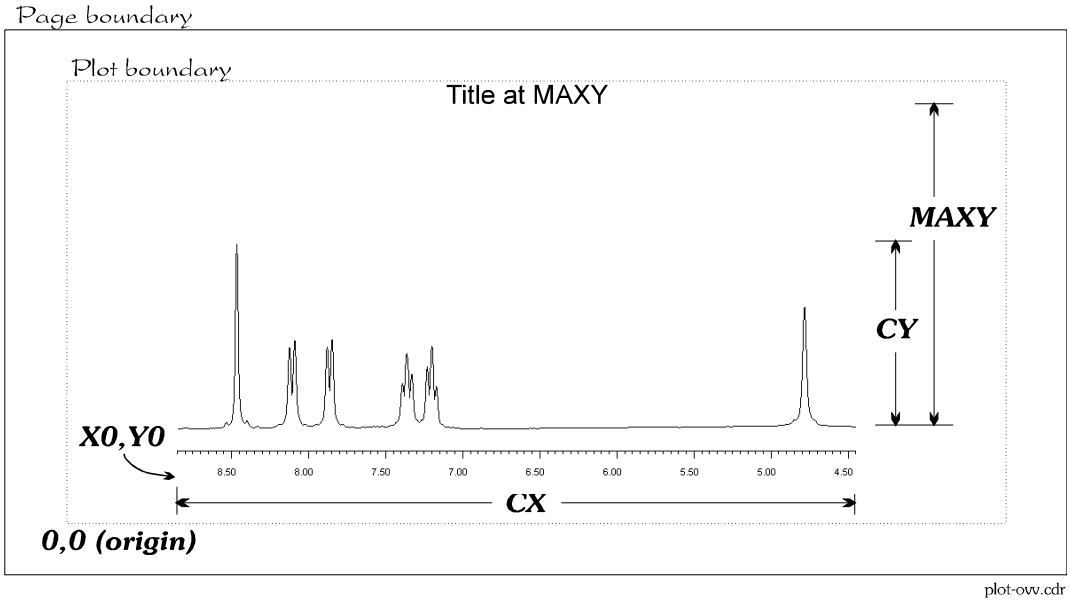
chose **LB** ~ –linewidth
chose **GB** ~ fraction AQ
where S/N first = 0

### *F. Common EP Commands*

**^B** – re-enable knobs A and B
**^F** – display current F1,F2 region
**^O** – set SW,O1 to expanded region
**^R** – display whole spectrum
**LINE FEED** – baseline points selection mode
**A** – add phase corrections
**B** – phase on biggest peak
**C** – phase on cursor selected peak
**D** – dual display
  **D** – decrease separation
  **I** – increase separation
  **S** – subtract spectra
**E** – toggle EP info. displays
**F** – enter frequency limits F1,F2
**G** – set spectrum reference (SR)
**H** – hard copy (print) cursor info.
**I** – enter integration mode
  **A** – calibrate (normalize) integrals
  **M** – toggle knobs C,D from cursor mode to slope and bias mode
  **S** – section plot of displayed integral
  **X** – full plot of displayed integral
  **Z** – zero integral; set starting-end points of integrals
**J** – enter line fitting mode
**K** – enter interactive baseline correction
**M** – set minimum intensity for peak picking
**P** – phase on biggest peak displayed
**O1** – printout absolute freq. of cursor
  **M** – will store frequency as O1
**O2** – printout absolute frequency of cursor
  **L** – stores freq to specified freq list file
  **M** – will store frequency as O2
**R** – use twice to set freq limits for expanded display (^B to reset A,B knobs)
**S** – section plot
**T** – enter cursor to T1PNTS file
**U** – update region for plotting
**X** – plot expanded region (PX)
**Y** – change CY,CX within EP
**<** – left shift one point (LS)
**>** – right shift one point (RS)
**:** – toggle
**5** – peak peak and display
**6** – move display down 1/8 screen
**7** – move display up 1/8 screen
**8** – display rms S/N
**9** – toggle to dots/connected display

## III. Plotting with DISNMR

### *A. Overview*




Plotting on Aspect computers starts similarly to any computer system, with page and plotting regions. The plotting region depends on the particular plotting device; here we'll assume either an HP LaserJet printer, or an HP 7475 or 7550A plotter. Landscape plotting is default on both plotters. The spectral region plotted is set with the **EP U** (update) command. Plot parameters can be read in with the **PJ** command (these jobfiles may not be present; we use NUTS to plot nearly all spectra):

| | |
|---|---|
| **PJ A3PLOT.1DJ** | 11×17" landscape plotting |
| **PJ A4PLOT.1DJ** | 8.5×11" landscape plotting |
| **PJ A3STKPLT.1DJ** | 11×17" stack plotting with rotated (portait) spectra |
| **PJ A4STKPLT.1DJ** | 8.5×11" stack plotting with rotated (portait) spectra |

The parameters and commands that control plotting (see figure above):

| Parameter/ Command | Description | Landscape 11×17" A3 | Landscape 8.5×11" A4 | Portrait 11×17" A3 | Portrait 8.5×11" A4 |
|---|---|---|---|---|---|
| X0 | X offset for origin | 0 | 0 | 0 | 0 |
| Y0 | Y offset for origin | 0-4 | 0-2 | 0-4 | 0-4 |
| CX | X-axis length of spectrum | 35 | 24 | 24 | 16 |
| CY | Height of reference (usually tallest) peak in spectrum | 20 | 16 | 30 | 20 |
| MAXY | Maximum Y deviation plotted | 22 | 18 | 32 | 22 |
| DPO rotate? | define plotter options | N | N | Y | Y |

### *B. Standard Plots*

1. **RE** spectrum in
2. **PJ** plot jobfile (see above)
3. check **DPO**, **CY**, and **MAXY**
4. **EP**, get spectrum on screen as wanting to plot and enter **U** to update plot region
5. use **X** and **S** inside EP, or exit EP and use **PX**
6. *remember to cap pens on pen plotters when finished*

### *C. Stack Plots*

1. Start by **RE**'ing bottom spectrum
2. **PJ** plot jobfile (see above)
3. check **DPO** (plot x-axis now, and rotate if want portrait stack), **CY**, and **MAXY** (title height)
4. check **X0,Y0** for initial plot (use **OP** if using **STACK.AU**; manual plotting is recommended)
5. use **EP** and **U** to update plot region; exit EP
6. plot first, bottom spectrum with axis and title using **PX**
7. **RE** next spectrum
8. change **DPO** for no axis or title plotting
9. increment **X0,Y0**
10. plot using **PX**
11. goto 9 and continue for all spectra
12. *remember to cap pens on pen plotters when finished*

## IV. Data Transfers

### *A. UW Network*

| | |
|---|---|
| Windows NT | - Backbone file server network for PC's |
| | - completely transparent to users, data is uplinked to a Snap server |
| NMR-Link | - Bruker file transfer network; bidirectional |
| | - writes files in Bruker image format (widely read by NMR software) |
| | - uses PC AT's to automatically send FASTRAN data to WinNT server |
| FTP | - File transfer protocol; generic file transfer between many platforms |
| NFS | - Sun's Network File system (must use FTP in our facility to transfer) |

(All FID files must be stored on AC spectrometer hard disk by using **WR <filename>** before the transfer.)

### *B. NMR-Link*

- NMR-Link exports and imports Bruker binary (and with a non-default setup, ASCII) data. The two commands used in this facility are:

  **topc** ***filename.ext*** to send files to the PC network

  **frompc** ***filename.ext*** to receive files from the PC network

  The above two commands are always issues while sitting at spectrometers or the datastation, with a PC-AT providing dedicated file servicing.

- ***NMR-Link at an AC Spectrometer***

  When at a spectrometer, the commands are run from the 2nd session, toggle to/from with the **<cntl>-X** command.

***C. FTP to/from NMRSnap***

- Login to NMRSnap.chem.wisc.edu from any FTP-capable computer (see postings in lab for password).

- The only directory that has write priviledges is \\nmrsnap\DataArchives\temp

## V. Formatting Floppy Disks

- Insert a blank 3-1/2" floppy disk in the disk drive and turn the drive ON. **MO** to exit to the monitor from DISNMR. **DSP ON** will toggle display to the monitor. Then, do as follows:

  ***ADAKET <ret>**
  SELECT FUNCTION? **F** (to format a floppy disk)
  ERASE DATA? **Y <ret>** ...formatting begins and takes ~45 seconds...
  **M** (to exit to the monitor)
  **DIR=F1** (to verify formatting)
  **LOAD ADAKOS**

- Reboot the computer by **STOP-CLEAR-DISK**. If DISNMR is not loaded automatically, type **DISR91**, followed by **<ret>**.