REMINDER SHEET FOR THE BRUKER AM-250

1. Insert Sample: Turn off *Spin* and *Lock*. *Lift*. Insert sample in spinner, adjust depth, wipe with ethanol-soaked Kim-Wipe, place on air cushion at top of bore. *Lift Off*. Set *Field*, *Lock Power*, *Lock Gain*, *Lock Phase* to card values for your solvent. Center signal (*Field*) and adjust height (*Lock Power* / *Lock Gain*) and symmetry (*Lock Phase*). Turn *Lock* and *Spin* on. Adjust *Z1* and *Z2* shims for maximum lock signal height.

2. Proton Acquisition:

RJ PROTON.xxx=D1	Recall standard ^{1}H parameters from disk: $CDCl_3$ solvent, xxx=CHL; D_2O = D2O; d_6-acetone = ACT; CD_3OD = MET; d_6-DMSO = DMS
II	Initialize the Interface for ^{1}H acquisition (Cap'n).
RGA	Receiver Gain Adjust - Automatic (wait for LCD message: Auto RG Finished)
NS	Set desired number of scans. 16 for most samples, increase for more dilute samples (in multiples of 8)
AI	Absolute Intensity (set to 0).
ZG	Acquire FID. Scan counter indicates progress, *Pulse* and *ADC* lights blink.

3. Carbon-13 Acquisition:

RJ CARBON.xxx=D1	Recall standard ^{13}C parameters from disk. See above for xxx.
DO *and* **II**	Gate the decoupler off and initialize the interface for ^{13}C acquisition
AU CARBON.AU=D1	Start ^{13}C acquisition (DO NOT USE ZG!!)
TR	Transfer FID to another job during acquisition
Cntrl-**H**	Stop ^{13}C acquisition when FID has sufficient signal-to-noise

4. Processing (common to ^{1}H and ^{13}C):

WR ***ABCD*xxxx.xxx=D2**	Save FID to disk. *ABCD* = first four letters of your login.
LB	Check Line Broadening: 0.2 (Hz) for ^{1}H, 1.0 (Hz) for ^{13}C
EF	Apply exponential multiplier and Fourier Transform.
EP	Enter interactive display mode: **A**, **B**, **C** and **D** knobs active. **A** moves display window left/right, **B** = width, **C** = cursor, **D** = fine cursor
P (With upfield region expanded)	Enter interactive Phasing routine:
	Adjust phase with **C** knob (*Cntrl*-**C** to extend knob range)
	Move display to downfield peaks with **A** knob
	Adjust phase of downfield peak with **D** knob (*Cntrl*-**D** to extend knob range)
M	Memory: Apply phase correction and exit Phasing routine.
On DOS PC at your left:	cd c:\data\zznet
	getzz
PASC SENDZZ	Enter filename (ABCDxxxx.xxx=D2) at the prompt

Control Commands:

Cntrl-**L**	Toggles between Lock Only, Spectrum/FID Only, and Both displayed
Cntrl-**D**	Toggles Grid Display On/Off
Cntrl-**H**	Abort acquisition
Cntrl-**E**	Abort any operation (Use if **PASC SENDZZ** fails)

5. Eject Sample and Insert Standard (1% $CHCl_3$ in $CDCl_3$, sealed tube). Lock and adjust lock settings.

6. Transfer FID to larmor and convert to XWinNMR format:

On DOS PC at your left:

```
cd  c:\data\zznet\data
ftp  larmor          (Enter login name and password)
bin                  (set to binary mode)
lls   ABCD*.*        (view list of your files on the DOS PC)
put   <filename>     (transfer FID to larmor)
quit                 (exit ftp)
```

On larmor (Linux PC farther to your left – log in with name and password):

```
convert              (run program to convert to XwinNMR format)
Enter AM-250 filename and new filename for XWinNMR
```

7. Process Your Data Using XWinNMR on larmor:

Fourier Transform: **>trf** (automatically switches display to spectrum window)
Position and Scale: **|<>|** full spectrum; ***2**, ***8**, **/2**, **/8** change vertical scale; move spectrum up and down.
Phase: Click **Phase**, **biggest** or **cursor**, **PH0** - drag up/down, **PH1** - drag up/down, **Return**, **Save and Return**.
Expand Region: Click on spectrum, click **middle mouse** in two places and then **left mouse** to get back **cursor**
Reference: Click on **Calibrate**, move **arrow** to top of reference peak and click **middle mouse**. Enter Shift.
Baseline Correction: **>abs** to automatically flatten the baseline (improves accuracy of integrals).
Integrate: Click on **Integrate**, click anywhere on spectrum and position **arrow,** click **middle mouse** to cut integral regions, click anywhere to get back cursor, click on **Return** and **Save as 'intrng' & Return**.
Peak Picking: **>pscal**, select **global**. Click **Utilities**, **Y** and **/** or **YU** to get vertical scale in cm, **Return**. Click **Analysis**, **Peak Picking** and **Adjust minimum intensity**, move horizontal line to desired threshold and click.

8. Plotting Your Spectrum:

Start: Click on **Windows** and **Plot editor** to Enter plotting program (XWinPlot)
Connect: Click on **XWIN-NMR** and **XWIN-NMR Interface**, **Create Parameter List**, and **Edit Title**. Click on **Create Peak List** (if you did Peak Picking in part 7 above), Click on **close**.
Spectrum: Click on Spectrum icon, position "+" cursor, click and drag to position spectrum on plot.
Parameters and Title: Click on icons, position cursor on plot and click. Click on **Attributes** to change font.
Adjust Spectrum: Click on *Mark Objects* icon, then on spectrum. Click on **1D/2D Edit**. Select **Show Peaks** and/or **Show Integrals** if desired, Click on **close**. Readjust spectrum size to fit in margins (dotted lines) using the green squares.
Plot Spectrum: Click on **File / Print**, **Print**. Click on **File / Close**, **OK** to exit Plot Editor.

9. Exit XWin-NMR and Log Out:

Click on **File / Exit**, **OK** to leave **XWin-NMR**. Click on Red Hat and **Logout**, **Logout** to confirm.

Do Not Logout From Linux Without First Exiting XWin-NMR!!! Do Not Exit XWin-NMR Using the Linux X on the Upper Right Corner!!! Any of these actions can leave processes "hung" and the next user will be unable to use the computer!!!