Quick Notes for Use of Bruker Avance Spectrometers at NMRFAM:

[cgfry: 99.04.12]

1. Use the Console window to start up xwinnmr: **xwinnmr**

2. Use an Xshell window to look at pulse sequences:
   cdpp
   vi *pulsesequence.cgf*
   (it is a good idea to copy the sequence to your initials; that gives you priviledges to comment and edit the sequence, since you will own it; use e.g., **cp *pulsesequence.*fa *pulsesequence.*cgf**)

   One can also use editors within xwinnmr by typing: **edprog**(?)
   The default editor that is used can be changed in **setres**.

3. Inside **setres** make sure to turn off *ZGsafe* (to 'no') as otherwise this will prevent **multizg** from continuing without user interaction (defeating the purpose of multizg).

4. To set the temperature, use:
   te↵ (enter new temp in kelvin)
   teset↵ (to force the change to the controller)

5. Lock using **lock**
   Select the solvent, and the spectrometer should lock up. Enter **lockdisp** to open the lock display window.

6. Once the lock settles (after a temp change), gradient shim by typing:
   gradshim↵

   A gradient shimming window will open; make sure the user is your id (e.g., *cgfry*) and not gradshim.

   Click on the **Start Gradient shimming** button, and wait until a graph comes up and the SGI finishes pushing the new shim values into the shim unit. At this point, the shims should be pretty good; you can play around with moving Z6 or Z5 significantly and re-gradient shimming to try to improve, or of course one could manually work on the shims.

   wsh and **rsh** work similarly to the AC/AM's, for writing and saving shims. However, once again Bruker forces all files from all users into a common directory, so make certain to append the suffix *.cgf* (use your own initials). That way:

   rsh **.cgf* will show just your shim files.

7. We have been using the following sequences:

zgpr.cgf	(poor quality presat—use ≤ 30dB—but ok for pw90 calibrations)
zg3919.cgf	(check quality and O1 setting for 3919 water suppression; p1 must be set = 90°)
roesy3919fa.cgf	(seems to be ok; spinlock power 15dB ~ 4kHz)
tocsy3919fa.cgf	(seems a problem with phase cycle; will recommend another when find one that works better)

You can see all pulse sequences by going into the **ased** window and clicking on the down arrow next to the pulsesequence. You can also change it directly by typing **pulprog↵** and typing in the new name.

8. Parameter sets can be read in to match the sequences listed above by typing:
   rpar *cgf (lists just subset written by cgfry)
   rpar (lists all parameters sets saved by any user)

   wpar will save your parameters; all files from all users go into a common directory, so append the suffix initials so you can isolate just your files with the first rpar command above

9. Old data sets can be read in by typing:
   dir and clicking on the desired set.

   In Unix, you can get to your dataset by typing: **cddata**
   The path is /u/data/cgfry/nmr or from a remote computer for the 750 /dmx750/data/cgfry/nmr

   Make new datasets, or new experiment numbers with:
   edc

10. Check the acquisition parameters by using:
    ased

    ased bring up a panel with pulse acquisition parameters specific to the pulsesequence chosen. If you change the pulse program within ased, exit and re-enter ased before changing other parameters.

    Then check other parameters for reasons unknown not included in ased using:
    eda

    o1, td1, nd0, and various other parameters have to be checked in eda or with the command line. Typically use **DQD**.

    It is recommended that the pulsesequence be open and checked while going through the parameters for the first time.

11. Check the gradient sequence using **grdprog** at the command prompt. Hopefully the sequence will have the name documented in the comment lines.

    Check **const21** etc. as required for the gradient sequence; follow comments in the pulseprograms.

12. Use **zg acqu** to start acquisition and switch to real-time fid observation to check the receiver gain level. Clipping occurs at the top and bottom of the unaltered acqu window (±12,000). For a 2D sequence, watch both the first and second rows, don't rely on just the first row as a check. For COSY-type sequences, change d0 ~ 10ms so the magnetization is echoing back for an rg check (remember to set d0 back after adjusting rg).

13. Backup data by using tar as usual, being careful to ***not*** include absolute paths in the input portion of the command:

    cddata
    tar cvf /shetland_data/*dir*/*tarfile.tar* *datasetname*

    From a remote computer, ftp or telnet can connect to hereford or shetland. Make sure to switch to binary transfer with **bin** before performing the ftp get command.

14. Use **edp** to process the data in xwinnmr. The comments in the pulse program will tell whether the data was acquired TPPI, States-TPPI, or States.

    xfb will transform in both directions keeping all quadrants of the data.
    xfb n will transform, but not keep the imaginary components; much faster, but you won't be able to phase without retransforming here.

    Use the +/- buttons to turn on negative and both signs of 2d sets.

    1d: use PHASE CUR and click middle button to define the toggle point, then click-hold the left button on PH0 and phase at the toggle point. Click-hold the left button on PH1 to 1st-order phase far away from the toggle point.

    pk will apply the previous phase correction

    2d: use PHASE CUR ROW and click middle button in 2d set; click on 1 to place in the 1 window; repeat for 2 and 3 windows. Then do PH0 and PH1.
    Repeat complete process for CUR COL if F1 needs phasing.

15. See the companion guide for information on how to translate the data into vnmr.