

Bruker AV500

computer name: ZMAN500

January 22, 2004, YB

1. Login and open the program

- sign the logbook
- bbi probe is in the magnet?
- type: rsh bbi <enter>
if you get some error message about the type of probe;
type: edhead <enter> and click on Define as current probe then Exit

2. Insert the sample

- use the ceramic rotor with the *yellow* stripe
- center the sample in the coil region (using the depth measure)
- press lift on/off
- cap the magnet bore

3. Set the sample temperature

- edte <enter>
- check that thermocouple, heater, and gas flow are attached
- ALWAYS use sufficient gas flow to prevent overheating!!!!
- limit high temperature runs according to the separate VT NMR instructions
- always minimize abrupt changes in temperature

4a. Create a file location for the data

- dir <enter>
- edc <enter> enter new expno click on save

4b. Read in experimental parameters

- rpar 1H_solids-bbi <enter>

5a. Create a file location for the data

- edc <enter> enter new expno click on save

5b. Read in experimental parameters

- rpar 47Ti_solids-bbi <enter>

6. TUNE and MATCH

- type atma in an expno with *parameters* for 47Ti acquisition to get the proper frequency

7. SWEEP OFF

- make sure the sweep button on the BSMS keypad is not lit = OFF

8. Acquire a FID:

- edc <enter> open the first expno in the series in the XWIN-NMR window
- check the temperatures in the vtlist:
 - type: edlist vt <enter>
 - click on the name of the vtlist
 - check and update file → save → exit
 - !note!** the temperature should start with the highest temperature and work down
 - do not run for too long a time at too high a temperature (expt <enter>)
 - ALWAYS have sufficient gas flow
- type: vtlist <enter>
 - enter the name of the vtlist
- check the receiver gain:
 - type: rg <enter> <enter>
 - type: rga <enter>
 - when finished, type: rg <enter>
 - if** the value of rg has changed
 - a) update all identical data sets
 - b) repeat the comparison for any other nuclei
 - c) **return to the first expno in the list before starting the acquisition**
- to run:
 - type: multi_zgvt <enter>
 - OK, OK, <enter>, 300 (5 minutes is 300 seconds) <enter>, etc.

 - to kill the run:
 - type: h <enter> if you want to save anything currently running
 - type: kill <enter>
 - select multi_zgvt and/or zg
 - repeat until nothing is running

 - to halt one expno, but continue with the series:
 - type: h <enter>

 - when** the last scan of the last expno in the series finishes,
you will get a message: **multi_zgvt finished**

9. Process and Plot:

- ef <enter>
- phase <enter>
 - click on biggest, adjust ph0, click on return, click on save and return
- abc <enter>
- click on dp1 to define the plot region
- click on utilities to interactively adjust CY (~13 cm) and MI, click on return
- view <enter> **or** open xwinplot (type: xwinplot <enter>)