Bruker AVANCE-360 User's Guide
for the UWChemMRF

by

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UWChemMRF User Guide for XwinNMR

I. Introduction

a) Account information

- passwd rules
  - do ***not*** use your email or 9th floor password; should be unique to CIC
  - use seven to eight characters, at least one non-alphanumeric
  - do not use any characters other than letters (case-sensitive), numbers, period, hyphen, underline
  - avoid simple substitutions: e.g., *b00tleg* is not a good password
- checkout requirements
  - all homework must be completed with 100% score before taking checkout
  - account locked-out one month after training if checkout not completed
  - account sharing will cause loss of access

b) Help

- See "The Interaction Between XwinNMR and Unix," pg. 4, 63 and 64
- All the Bruker manuals are accessible at the spectrometer under the XwinNMR Help menu.
- All the Bruker manuals are accessible on-line from our home page:

  go to: http://cic.chem.wisc.edu/nmr/main.html
  find: User Guides
  click on: Bruker AVANCE User Guides
- These documents are available in the same area of the web site.

Use the on-line and printed help manuals often and regularly. Asking questions prior to your having looked first yourself will not be well-tolerated.

c) Natoth SGI Unix – brief intro

- See "The Interaction Between XwinNMR and Unix," Part I; especially pgs. 5-7, 15-18, and 27-30 (note: much of the rest requires root privileges)
- .cshrc and aliases

dir	; **ls –laF** (at UNIX prompt only; different in Xwin)	
df –k	; check disk utilization	
cd	; standard csh—puts in home directory	
cddata	; only cd alias that is user specific	pg 79-80
cdshims	; shims directory	pg 70
cdpp	; pulse programs	pg 71
cdpar	; parameter files	pgs 69, 84
cdmac	; macros (simple command execution)	pg 70, 90
cdau	; automation files (c-like)	pg 69, 85-89
cdgp	; gradient programs	missing on pg 69

d) File structures and naming conventions

- See "The Interaction Between XwinNMR and Unix," Part II; pgs 66, 69, 70

Filenames	14 letter limitation; edc
Data locations and structure	pgs 79-80
Shim files	pg 70
Parameter files	pgs 69, 84
Pulse programs	pg 71
Macro files	pgs 70, 90
Automation files	pgs 69, 85-89

e) XwinNMR and setres

- See "The Interaction Between XwinNMR and Unix," Part II; pg 91

ZGSafety	; 'yes' initially, but *must* be set 'no' for **multizg**
Default Editor	; use "jot"
XwinNMR	; set to "Extended"
Apply	; will correct color/display problems

f) Editors

- See "The Interaction Between XwinNMR and Unix," pg. 72, 79

edc	; edit current (for new data acquistion)
eda	; edit acquisition parameters
ased	; automation setup editor (pp dependent)
setti (edti; UW macro; also edinfo)	; edit title (useful for data commenting)
edte	; edit temperature (temp panel)
edhead	; edit probehead (for probe changes)
edp	; edit processing parameters
edg	; edit plotting parameters

g) Modern High-Field Spectrometers

Linear Amplifiers ; see edacb

Bruker (stated in attenuation, not power!!)		Varian
-6dB	high power proton bb probes	63
0dB	high power X	58
≤30dB	presaturation	24
≤40dB	homodecoupling	18
≤16dB	highpower decoupling	41
≤10dB	highpower spinlock (check for update before using)	41

Tuning probes ; see Acquisition Manual 1.5.4, pg A-60

wobb	; needed for changes in temp for 1H ; required for all X-nucleus experiments
wob	; UW macro, does an acqu prior to wobb

h) Starting and Stopping Acquisitions

- See "XwinNMR Acquisition Manual," Section 1.7
- do **not** use quicknmr or run (they are not setup)

```
zg        ; zero data then go
go        ; do not zero data (ie., add to current)
tr        ; transfer data for processing
halt      ; preferred method for ending acquisition
stop      ; immediate termination of acquisition, not as safe as halt
suspend   ; suspend and resume only if pulse program supports (usually not)
resume    ; resume only if supported in pulse program
kill      ; will terminate active processes (e.g.,
```

i) Plotting Data

- See "XwinPLOT manual" on cic website
- PLOT button works fine in XwinNMR (but pretty limited)
- type xwinplot to start up very nice plot editor
  - main customization is *right-click* on object and select *1D-2D-edit*