V. VNMR to Bruker-AM/AC Parameter Conversion Table

[comments apply to VNMR unless specifically mentioned otherwise]

Parameter	AM/AC	VNMR	Comments
Experiments			
standard 1d ^{1}H	**ZG**	**go / s2pul**	go zeros memory, and starts acquisition; seqfil='s2pul'
homonuclear decoupling	**HOMODEC.AU**	**s2pul homo='y'**	set the cursor on the peak and use **sd** to get the decoupler frequency
1d NOE difference	**NOEDIFF.AU**	**s2pul homo='y' dm='yyn'**	array can be used to run multiple decoupler frequencies in one exp.
standard 1d decoupled $X/^{13}C$	**CPD ZG**	**s2pul dm='yyy'**	
NOE-enhanced coupled ^{13}C	**GATEDEC.AU**	**s2pul dm='yyn'**	DEPT is preferred unless you need quat's
quantitative decoupled ^{13}C	**INVGATE.AU**	**s2pul dm='nny'**	*X* nucleus T_1's can be quite long, so this experiment can be arduous
DEPT ^{13}C editing	**DEPT.AU**	**dept**	mult=0.5; 1; 1.5 produces dept45; 90; 135 respectively
homonuclear correlation 2d	**COSY.AU**	**cosy**	gcosy is the better experiment; sw/(ni*2) gives usable digital resolution; usually need ≤ 6 Hz/pt
long-range cosy	**COSYLR.AU**	**cosy tau≠0**	gcosy is the better experiment
double quantum cosy	**DQCOSY.AU**	**dqfcosy**	DQCOSY; complete phase cycling is crucial for the dq filter; nt = multiple of 8
phase sensitive noesy	**NOESYPH.AU**	**noesy**	NOESY: flat baselines are important for observing small noe's; use **calfa**
phase sensitive roesy	**ROESYPH.AU**	**roesy**	ROESY; flat baselines are important for observing small noe's; use **calfa**
total correlation/WOHAHA	**???**	**tocsy**	TOCSY or TOCSY1D; useful for mixtures or separated spin systems
heteronuclear correlation	**XHCORR.AU**	**hetcor**	use only if need very high ^{13}C resolution
inverse hetero correlation	**???**	**hmqc**	gHMBCAD preferred
multiple bond hetero correl.	**???**	**hmqc bond≠0**	HSQCAD; important experiment for observing through linkage bonding

Read and Save Commands			
read data file	**RE *filen.ame***	**rt('*filename*')**	in VNMR, use also MAIN MENU FILE click on filename and LOAD
save data file	**WR *filen.ame***	**svf('*filename*')**	in VNMR, no menu selections for this
read parameter file	**RJ *filen.ame***	**rtp('*filename*')**	in VNMR, use also MAIN MENU SETUP NUC,SOLV
save parameter file	**WJ *filen.ame***	**svp('*filename*')**	
read shim file	**RSH *filen.ame***	**rts('*filename*')**	in VNMR, will search ~/vnmrsys/shims and /vnmr/shims paths
save shim file	**WSH *filen.ame***	**svs('*filename*')**	in VNMR, will save to ~/vnmrsys/shims
load shim file	none needed	**loadshims**	loadshims is UW-written macro having **load='y' su load='n' su**

1d Acquisition Commands			
tune ^{1}H observe	**RJ H1.SET**	**UWmacro TuneH1**	tuneh is a UW-written macro
tune ^{13}C channel	**RJ C13.SET**	**UWmacro TuneC13**	tunec is a UW-written macro
setup 1H for CDCl3	**RJ CDCL3.1DJ**	use menus	in VNMR, use MAIN MENU SETUP NUC,SOLV
zero and go	**ZG**	**go** or **ga**	**ga** will automatically apply a **wft** after acquisition
automation run	**AU *autom.nam***	**au**	all VNMR programs run from compiled routines
halt acquisition with data	**^H**	**sa**	in VNMR, svf can be issued during acquisition to save data
resume acquisition	**GO**	**ra**	seems to work only for 1d (unless the 2d or 3d has been modified); vnmr's **ra** follows an **sa** that stops acq.
abort acquisition	**^E** or **^K**	**aa**	in VNMR, data is retained and ok
automation setup	**AS *auton.ame***	none (try **dps**)	in VNMR, only parameters used in experiment will be shown
1d Acquisition Parameters			
sweep width	**SW**	**sw**	
center or offset frequency	**O1**	**tof**	
center decoupler freq	**O2**	**dof**	
solvent	none (change O1 thru jobfile)	**solvent='cdcl3'**	with solvent set correctly in VNMR, **tof=0** will center spectrum for normal organic compounds

set spectrum window	**EP** set window **^O**	set cursors **movesw**	changes **SW, O1** → **sw, tof** ; on Brukers, **AQ** will change, whereas in VNMR, **np** will change (leaving **at** unchanged)
set offset frequency	**EP** set cursor **O1**	set cursor **movetof**	changes **O1** → **tof**
relaxation delay	**RD** or **D1**	**d1**	AM/AC delay differs depending on ZG or AU to run experiment
common pulse width	**PW**	**pw**	90° length fixed by probe on AM/AC's; depends also on **pw90** and **tpwr** in VNMR
acquisition time	**AQ** (=TD*DW)	**at** (=np/sw)	
dwell time	**DW** (=1/(2*SW)	= 1/sw	Bruker acquires complex pairs sequentially, vnmr simultaneously
# of transients to acquire	**NS**	**nt**	Bruker NS -1 which goes continuously → vnmr nt=1e6
# transients before acquis.	**DS**	**ss**	
receiver gain	**RG** (larger # → larger gain)	**gain** (larger # → larger gain)	on Unity, if gain=0 still clips (get ADC OVERFLOW message), insert attenuator at preamp output
observe transmitter power	none	**tpwr=52** (higher # → higher power)	AM/AC's observe power is fixed; Unity's have linear amplifiers on both observe and decouple
number of points acquired	**TD** (usually = SI)	**np**	
temperature	**TE**	**temp=24**	see **temp24** and similar macros (written at UW)
decoupler transmitter power	**DP<ret>20H** (lower # → higher power)	**dpwr=40** (lower # → lower power)	vnmr parameters are logical

1d Processing Commands and Parameters			
fourier transform	**FT**	**ft**	
number of points FT'd	**SI**	**fn**	zero-filling occurs here (e.g., np=1024, fn=2048 will zero-fill once)
line broadening parameter	**LB**	**lb**	
interactively set weighting parameters	none	**wtia** or **wti**	in vnmr, middle button still control intensity in all windows; left button sets parameter
apply exponential line broad.	**EF**	**wft** or **dsx**	in vnmr, **wft** applies whatever weighting function is setup; **dsx** is a UW macro, and simply adds a **dscale(0)** after the FT

set reference	**EP** set cursor **G**	set cursor **nl** **rl(0p)**	vnmr gives example for TMS
automatic phasing	**AZPK??**	**aph**	in vnmr, **lp** should ~ 0, otherwise advise **calfa** command and/or back-linear prediction
baseline correction	**EP K**	**dc** or **bs(5)**	in vnmr, **bs** is *not* recommended for 1d (default spline fit), but is very good for 2d work-ups (recommended there)
normalized intensities	**AI<ret>0**	**nm**	in vnmr, vs=100 will fill screen
absolute intensities	**AI<ret>1**	**ai**	
1d Plotting Commands			
plot spectrum	**PX**	**pl**	
plot parameters	in **DPO** setup	**ppa** or **pap**	
plot axis	in **DPO** setup	**pscale**	in vnmr, axis='p' sets axis to ppm
plot coordinates	**X0, Y0**	**sc, vp**	sc is mm from right side, vp is mm vertically up from bottom
plot size	**CX, CY**	**wc, vs**	wc is mm width of chart, vs is vertical scale
plot integrals	**PXD???**	**pirn**	
plot peak picks	in **DPO** setup	**dll** or **ppf**	**printon dll printoff** prints table to separate page (do before any plotting commands); **ppf** plots on spectrum
new page	**NP**	**page**	

2d Acquisition Parameters			
sweep width for F1	**SW1**	**sw1**	AC/AM SW1 is 1/2 of observed sweep width; vnmr sw1 = observed sweep width
# increments/experiments	**IN**	**ni**	in vnmr, phase determines total # experiment = 1× or 2×ni
type of 2d acquisition	**MC2**	**phase**	AC/AM: only absolute value and TPPI are available in software vnmr: absolute value → phase=0 States-Habercorn → phase=1,2 TPPI → phase=3
2d setup	**ST2D**	none	in vnmr, type in sequence macro then **dps**
total time of experiment	none	**time**	
interleaved acquisition	depends on routine	**il='y'**	in vnmr, acquire **bs** scans per increment, loop until **nt** completed
2d Processing Commands and Parameters			
FT size in F1	**SI1**	**fn1**	AC/AM square requires SI1=SI/2=SI2/2
reference in F1	**SR1**	set cursor, **rl1(0p)**	
FT and weight full set	**XFB**	**wft2da**	in vnmr, for absolute value sets use **do2d** or **wft2d**
FT and weight t_2 dimension	**XF1**	**wft1da**	counter-intuitive commands, but mean 1st transform
interactive weighting	none	**wtia**	can be done on t_2 fid, e.g., **wft(1) wtia**, and on t_1 fid, e.g., **wft1da TRACE wtia**
display color map	**EP2D** or **AP2D**	**dconi**	
2d Plotting Commands			
plot contours	**CPL**	**pcon**	in vnmr, see also **pconpos** and **pconneg**, UW written macros
plot size	**CX, CY**	**wc, wc2**	in vnmr, sc still controls distance in mm from right-hand side
Plot 2d using high res 1d		**plot2dhr**	have 1d high res already worked up in separate exp, follow prompts
peak picking and volumes	none	**ll2d**	