APPENDIX A ^{13}C ssNMR programme command

Appendix A1   CPMAS pulse programme command

\# 1 "/opt/topspin/exp/stan/nmr/lists/pp/user/cf.cp"
;cf.cp (TopSpin 2.0)

;based on cp experiment

;Avance II+ version
;parameters:
;p3 : proton 90 at power level pl2
;p15 : contact time at pl3 (f1) and pl4 (f2)
;pl3 : X power level during contact
;sp0 : proton power level during contact
;pl2 : power level proton pulse
;pl12 : decoupling power level (if not pl13)
;pl13 : special decoupliong power level
;d1 : recycle delay
;pl1: power level X pulse
;p1 : optional X pulse
;pl4 : proton power level during contact
;cnst21 : on resonance, usually = 0
;pcpd2 : pulse length in decoupling sequence
;cpdprg2 : cw, 1 (at pl12), or lgs, cwlg. cwlgs (LG-decoupling
;spnam0 : use e.g. ramp.100 for variable amplitude CP
;here pl13 is used instead of pl12)
;zgoptns : -Dfslg, -Dlacq, or blank

;$COMMENT=basic cp experiment, arbitrary contact and decoupling schemes
;$CLASS=Solids
;$DIM=1D
;$TYPE=cross polarisation
;$SUBTYPE=simple 1D
;$OWNER=Bruker
prosol relations=<solids_cp>

\# 1 "/opt/topspin/exp/stan/nmr/lists/pp/Avancesolids.incl" 1
;Avancesolids.incl
;   for 1
;
;version 1 28.2.2001, written by HF
;   4.4.2006, complemented by Ste

;$COMMENT=definitions for setrtp and setnmr
;$CLASS=Solids INCL

;switch between 1H or 19F output (H amplifier)
;$OWNER=nmrsu

;gating pulse for RX, ADC and HPPR auto mode

;explicit blanking of preamp, receiver, adc, not implemented yet

;generate dwell clock

;turn dwell clock on/off
;

;define data sampling for WAHUHA type experiments, samples analogue or digitally
for d9, closes receiver

;explicit transmitter blanking, not supported yet

;NCO switching, to be implemented
33 "/opt/topspin/exp/stan/nmr/lists/pp/user/cf.cp" 2

;cnst11 : to adjust t=0 for acquisition, if digmod = baseopt
"acqt0=1u*cnst11"

1 "mc_line 46 file /opt/topspin/exp/stan/nmr/lists/pp/user/cf.cp dc-measurement
inserted automatically"
    dccorr
46 "/opt/topspin/exp/stan/nmr/lists/pp/user/cf.cp"
1 ze

2 d1 do:f2
1 "/opt/topspin/exp/stan/nmr/lists/pp/p15_prot.incl" 1
;p15_prot.incl

; Test the rf on-time and duty cycle
;protect against too long contact time
;Test the rf on-time and duty cycle
;$COMMENT=protect against too long contact time
;$CLASS=Solids INCL
;$OWNER=nmrsu
1m
if "p15<10.1m" goto Passp15
print "contact time exceeds 10msec limit!"
goto HaltAcqu
Passp15, 1m

49 "/opt/topspin/exp/stan/nmr/lists/pp/user/cf.cp" 2

                          ;make sure p15 does not exceed 10 msec
                          ;let supervisor change this pulseprogram if
                          ;more is needed

                          ;disable protection file for long acquisition change decoupling
power !!! or you risk probe damage
                          ;if you set the label lacq (ZGOPTNS -Dlacq), the protection is
disabled

```
;#include <aq_prot.incl>
                           ;allows max. 50 msec acquisition time, supervisor
                           ;may change  to max. 1s at less than 5 % duty cycle
                           ;and reduced decoupling field


  10u pl2:f2 pl3:f1
  1u fq=cnst21:f2
  (p3  ph1):f2
  (p15 ph2):f1 (p15:spf0 pl4 ph10):f2
3 2u pl1:f1
  (p1 ph4):f1
 lo to 3 times l0
  2u pl12:f2
  go=2 ph31 cpds2:f2          ;pl12 is used here with 1, pl13 with cwlg, cwlgs
  1m do:f2
  wr #0
HaltAcqu, 1m
exit

ph0= 0
ph1= 1 3
ph2= 0 0 2 2 1 1 3 3
ph4= 1 1 1 1 2 2 2 2
ph10= 0
ph31= 0 2 2 0 1 3 3 1
```

Appendix A2 DP SatRec pulse programme command

1 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d"
;ch.satrect_2d (TopSpin 2.0)

;based on BRRUKER saturation recovery T1 experiment
;written by STE, 28.11.2002
;pulse program is for 2D acquisition
;establish suitable vd list
;uses mc syntax, so that it can be used in 1D mode for set-up of
;saturation pulse train

;Avance II+ version
;parameters:
;d1 : recycle delay
;d20 : delay in saturation pulse train
;l20 : number of pulses in saturation pulse train, 0 if undesired
;vdlist : list containing tau delays
;p1 : X 90 degree pulse
;pcpd2 : pulse length in decoupling sequence
;pl1 : X power level
;pl2 : =119 dB, not used
;pl12 : power level for H 90 and standard proton decoupling
;pl13 : e.g. used in tppm13
;FnMode : QF
24 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d"
;$COMMENT=saturation recovery T1 experiment
;$CLASS=Solids
;$DIM=pseudo 2D
;$TYPE=direct excitation
;$SUBTYPE=T1/T2

;$OWNER=Bruker
;cnst11 : to adjust t=0 for acquisition, if digmod = baseopt
"acqt0=1u*cnst11"

1 "mc_line 34 file /opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d dc-
measurement inserted automatically"

    dccorr
34 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d"
1 ze
2 d1 do:f2   ;recycle delay, decoupler off in go-loop
37 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d"
3 (p1 pl1 ph4):f1
 d20
 lo to 3 times l20
 vd   ;recovery delay
 (p1 pl1 ph1):f1

 0.1u pl12:f2
 go=2 ph31 cpds2:f2

```
  1m do:f2
  30m wr #0 if #0 zd
  ivd
  lo to 2 times td1

exit
# 52 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.satrect_2d"
ph1= 0 0 2 2 1 1 3 3
ph4= 0
ph31= 0 0 2 2 1 1 3 3
```

1 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d"
;ch.invrec_2d (TopSpin 2.0)

;based on BRRUKER saturation recovery T1 experiment
;written by STE, 28.11.2002
;pulse program is for 2D acquisition
;establish suitable vd list
;uses mc syntax, so that it can be used in 1D mode for set-up of
;saturation pulse train

;Avance II+ version
;parameters:
;d1 : recycle delay
;d20 : delay in saturation pulse train
;l20 : number of pulses in saturation pulse train, 0 if undesired
;vdlist : list containing tau delays
;p1 : X 90 degree pulse
;pcpd2 : pulse length in decoupling sequence
;pl1 : X power level
;pl2 : =119 dB, not used
;pl12 : power level for H 90 and standard proton decoupling
;pl13 : e.g. used in tppm13
;FnMode : QF
24 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d"
;$COMMENT=saturation recovery T1 experiment
;$CLASS=Solids
;$DIM=pseudo 2D
;$TYPE=direct excitation
;$SUBTYPE=T1/T2

;$OWNER=Bruker
;cnst11 : to adjust t=0 for acquisition, if digmod = baseopt
"acqt0=1u*cnst11"
"p4=2*p3"

1 "mc_line 35 file /opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d dc-measurement inserted automatically"

   dccorr
35 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d"
1 ze
2 d1   ;recycle delay, decoupler off in go-loop
38 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d"
 (p4 pl1 ph4):f1
  vd   ;recovery delay
 (p3 pl1 ph1):f1
  go=2 ph31
  30m wr #0 if #0 zd
  ivd
  lo to 2 times td1

exit

ph1= 0 2 2 0 1 3 3 1
ph4= 0
ph31= 0 2 2 0 1 3 3 1
# 52 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/ch.invrec_2d"
;p3 : pi/2 1H pulse
;p4 : pi 1H pulse calculated

```
# 1 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new"
;cf_torchia_2d
; based on cp.av basic cp experiment

prosol relations=<solids_cp>
# 1 "/opt/topspin3.0/exp/stan/nmr/lists/pp/trigg.incl" 1
;$COMMENT=definition of external trigger output, conn I pin 1
;$CLASS=Solids INCL
;$OWNER=nmrsu

# 5 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new" 2

;10 usec trigger pulse at TCU connector I cable 6

"p30=p31-0.4u"  ;calculate correction for last TPPM/SPINALn pulse
# 1 "mc_line 10 file /opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new dc-
measurement inserted automatically"

    dccorr
# 10 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new"
# 10 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new"
1 ze   ;accumulate into an empty memory

2 d1 do:f2 ;recycle delay, decoupler off in go-loop#include <p15_incl.prot>

;make sure p15 does not exceed 10 msec
# 1 "/opt/topspin3.0/exp/stan/nmr/lists/pp/aq_prot.incl" 1
;aq_prot.incl
; Test the rf on-time and duty cycle
;protect against too long acquisition time
;$COMMENT=protect against too long acquisition time
;$CLASS=Solids INCL
;$OWNER=nmrsu
1m
if "aq<50.1m" goto Passaq
print "acquisition time exceeds 50m limit!"
goto HaltAcqu
Passaq, 1m
# 15 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new" 2

;make sure aq does not exceed 50 msec

  1u fq=cnst21:f2
  10u pl2:f2 pl3:f1 ;preselect pl12 drive power for F2, pl3 for F1
  6u setnmr3|28 \n 4u  setnmr3^28   ;trigger for scope, 10 usec

  p3:f2 ph1  ;proton 90 pulse
  0.3u
  (p15 ph2):f1 (p15:sp0 ph10):f2 ;contact pulse with square or ramp
  1u pl1:f1
```

```
  (p1 ph4):f1

  vd
  (p1 ph5):f1 ; Laenge p5 mit Phase 5 auf X
# 31 "/opt/topspin3.0/exp/stan/nmr/lists/pp/user/cf_torchia_2d_new"
  0.5u pl12:f2
  0.5u cpds2:f2
  go=2 ph31     ;p31 used here case of TPPM/SPINALn
  1m do:f2  ;decoupler off
  30m wr #0 if #0 zd   ;save data to disk
  ivd
  lo to 2 times td1
HaltAcqu, 1m  ;jump address for protection files
exit   ;quit

ph0= 0
ph1= 3 1
ph2= 3
ph4= 2
ph5= 3 3 0 0 1 1 2 2
ph10= 0
ph31= 0 2 1 3 2 0 3 1

;cpdprg2:cw, TPPM, or SPINALn (at pl12)
;l1:switch on optional f1 store pulse
;pl1:f1 power level for (optional) pulse
;pl2:f2 power level for p3
;pl3:f1 power level for CP
;pl4:f2 power level for CP
;pl12:f2 power level for decoupling
;p1:f1 pulse for calibration at pl1
;p3:proton 90 at pl2
;p15:contact time at pl1 (f1) and pl2 (f2)
;p31:TPPM/SPINALn pulse
;cnst21:f2 frequency offset
;l0:optional f1 pulse for calibration
```