

Pseudo-3D Modulated HETCOR pulse sequence

Used on Bruker 600 MHz and 900 MHz instruments with DCH and TCO probes, respectively.

TopSpin software version 4.0.4

```
;hetcor.jmod.pseudo3D.110518.rw
;avance-version (11/05/18)
;2D heteronuclear shift correlation
;with refocussing of chem. shifts and
;phase sensitive
;
;
;CLASS=HighRes
;DIM=
;TYPE=
;SUBTYPE=
;COMMENT=

#include <Avance.incl>
#include <Delay.incl>
#include <Grad.incl>

"p2=p1*2"
"p4=p3*2"
"d11=30m"
"d12=20u"

; 1H delay
"d0=3u"
; Jmod delay
"d10=2m"

; 1H delay increment
"in0=inf1/2"
; Jmod delay increment
"in10=14/15000"

"d4=2*d5+p4-d10"

1 ze
2 d11
3 d1 do:f2
  d12 p12:f2 UNBLKGRAD
  ; Saturate Equilibrium Carbon Magnetization
  p1
  p16:gp1
  d16
; Proton Evolution
  (p3 ph1):f2
  d0
  p1 p2 ph4 p1
  d0
; Constant-Time J-Modulation during INEPT transfer to Carbon
  (center (d5 p4 ph2 d5):f2 (d4 p2 ph2 d10))
  (p3 ph3):f2 (p1 ph5)
; Refocus antiphase carbon to in-phase
  d3
  (center (p4 ph2):f2 (p2 ph6) )
  d3 p112:f2 BLKGRAD
; acquisition with 1H decoupling
  go=2 ph31 cpd2:f2
  d11 do:f2 mc #0 to 2
  F1PH(caliph(ph3, +90), caldel(d0, +in0))
  F2QF(caldel(d10,+in10), caldel(d4,-in10))
```

exit

ph1=0  
ph2=0 0 2 2  
ph3=1 3  
ph4=1 1 3 3  
ph5=0 0 0 0 1 1 1 1 2 2 2 2 3 3 3 3  
ph6=0 0 2 2 1 1 3 3  
ph31=0 2 0 2 1 3 1 3 2 0 2 0 3 1 3 1

;p11 : f1 channel - power level for pulse (default)  
;p12 : f2 channel - power level for pulse (default)  
;p112: f2 channel - power level for CPD/BB decoupling  
;p1 : f1 channel - 90 degree high power pulse  
;p2 : f1 channel - 180 degree high power pulse  
;p3 : f2 channel - 90 degree high power pulse  
;p4 : f2 channel - 180 degree high power pulse  
;d0 : incremented delay (2D) [3 usec]  
;d1 : relaxation delay; 1-5 \* T1  
;d3 : refocusing delay [0.8 msec]  
;d4 : decremented modulation delay  
;d5 : proton delay; T/2  
;d10: incremented modulation delay  
;d11: delay for disk I/O [30 msec]  
;d12: delay for power switching [20 usec]  
;d16: gradient recovery  
;inf1:  $1/SW(H) = 2 * DW(H)$   
;in0:  $1/(2 * SW(H)) = DW(H)$   
;nd0: 2  
;ns: 2 \* n  
;ds: 16  
;td1: number of experiments  
;FnMODE: States-TPPI, TPPI, States or QSEQ  
;cpd2: decoupling according to sequence defined by cpdprg2  
;pcpd2: f2 channel - 90 degree pulse for decoupling sequence

;\$Id: hxinepph,v 1.8 2012/01/31 17:49:26 ber Exp \$

```
##TITLE= Parameter file, TopSpin 4.0.4
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 526 $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= rvwillia
$$ 2018-11-14 16:24:08.399 -0500 rvwillia@br900
$$ /opt/nmrdata/rvwillia/13C-Me-Val-Robo1+Dy/7/acqus
$$ process /opt/topspin4.0.4/prog/au/bin/sertoint
##$ACQT0= 0
##$AMP= (0..31)
100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100
100 100 100 100 100 100 100 100 100 100 100 100 100 100
##$AMPCOIL= (0..32)
-1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_getlinv>
##$AUTOPOS= <>
##$BF1= 226.252375
##$BF2= 899.79
##$BF3= 899.79
##$BF4= 899.79
##$BF5= 899.79
##$BF6= 899.79
##$BF7= 899.79
##$BF8= 899.79
##$BWFAC= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$BYTORDA= 0
##$CAGPARS= (0..11)
0 0 0 0 0 0 0 0 0 0 0
##$CHANFCU= (0..24)
0 1 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$CHANREC= (0..24)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$CHEMSTR= <none>
##$CNST= (0..63)
1 1 125 1 1 1 1 1 1 1 6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$CPDPRG= (0..8)
<> <> <garp> <> <> <> <> <>
##$D= (0..63)
3e-06 1.5 0 0.0008 0.0300238 0.016 0 0 0 0 0.002 0.03 2e-05 0 0 0 0.0002
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0
##$DATE= 1542230654
##$DE= 33.75
##$DECBNUC= <off>
##$DECIM= 5400
##$DECNUC= <off>
##$DECSTAT= 4
##$DIGMOD= 3
##$DIGTYP= 17
##$DQDMODE= 0
##$DR= 32
##$DS= 16
##$DSPFIRM= 1
##$DSPFVS= 21
##$DTYPA= 0
##$EXP= <HSQCGPPH>
##$FCUCHAN= (0..9)
0 3 1 0 0 0 0 0 0 0
```

```
##$FL1= 0
##$FL2= 0
##$FL3= 0
##$FL4= 0
##$FN_INDIRECT= (0..7)
0 1 2 0 0 0 0 0
##$FOV= 0
##$FQ1LIST= <>
##$FQ2LIST= <>
##$FQ3LIST= <>
##$FQ4LIST= <>
##$FQ5LIST= <>
##$FQ6LIST= <>
##$FQ7LIST= <>
##$FQ8LIST= <>
##$FS= (0..7)
83 83 83 83 83 83 83 83
##$FTLPGN= 0
##$FW= 2.4e+08
##$FnILOOP= 0
##$FnMODE= 0
##$FnTYPE= 0
##$GPNAM= (0..31)
<> <SMSQ10.100> <SMSQ10.100> <SMSQ10.100> <> <> <> <> <> <> <> <> <> <>
<> <> <> <> <> <> <> <> <> <> <> <> <> <> <> <>
##$GPX= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPY= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GPZ= (0..31)
0 80 30 20.1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$GRPDLY= 76
##$HDDUTY= 20
##$HDRATE= 1
##$HGAIN= (0..3)
0 0 0 0
##$HL1= 0
##$HL2= 0
##$HL3= 0
##$HL4= 0
##$HOLDER= 0
##$HPMOD= (0..32)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$HPPRGN= 0
##$IN= (0..63)
0.0001852 0 0 0 0 0 0 0 0 0 0.00093335 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0
##$INF= (0..7)
0 370.4 111.2 0 0 0 0 0
##$INP= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$INSTRUM= <CAB AV4 900 MHZ EXT>
##$INTEGFAC= (0..63)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$L= (0..31)
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##$LFILTER= 50
##$LGAIN= -9.39999961853027
##$LNPSTP= 0
##$LOCKED= yes
##$LOCKFLD= -1133
##$LOCKGN= 115.564682006836
```

```
##$LOCKPOW= -18
##$LOCKPPM= 4.69999980926514
##$LOCNUC= <2H>
##$LOCPHAS= 293.0856
##$LOCSHFT= yes
##$LOCSW= 0
##$LTIME= 0.46399998664856
##$MASR= 5000
##$MASRLST= <masrlst>
##$MULEXPNO= (0..15)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$NBL= 1
##$NC= -7
##$NLOGCH= 4
##$NOVFLW= 0
##$NS= 92
##$NUC1= <13C>
##$NUC2= <1H>
##$NUC3= <off>
##$NUC4= <off>
##$NUC5= <off>
##$NUC6= <off>
##$NUC7= <off>
##$NUC8= <off>
##$NUCLEUS= <off>
##$NUSLIST= <automatic>
##$NusAMOUNT= 50
##$NusFPNZ= no
##$NusJSP= 0
##$NusSEED= 54321
##$NusSPTYPE= 0
##$NusT2= 1
##$NusTD= 0
##$O1= 4185.6689375
##$O2= 899.789999948553
##$O3= 0
##$O4= 0
##$O5= 4229.02
##$O6= 4229.02
##$O7= 4229.02
##$O8= 4229.02
##$OVERFLW= 0
##$P= (0..63)
12 12 24 11.9 23.8 16.5 25 50 273 20 40 40000 40000 2000 0 0 1000 2000
500 600 2500 0 0 0 1000 0 500 12 0 2000 0 0 2467 0 0 0 80000 0 0 1133 4000
0 0 10000 493 0 40000 700 1333 0 40000 0 0 0 0 0 0 0 0 0 0 0 0 0 933
##$PACOIL= (0..32)
3 4 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PAPS= 0
##$PARMODE= 2
##$PCPD= (0..9)
0 45 65 0 0 0 0 0 0 0
##$PEXSEL= (0..9)
1 1 1 1 1 1 1 1 1 1
##$PHCOR= (0..31)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PHLIST= <>
##$PH_ref= 0
##$PL= (0..63)
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120
##$PLSTEP= 0.1
##$PLSTRT= -6
```

```
##$PLW= (0..63)
0 51.394 20.606 0 0 0 0 0 0 11.841 0.47365 0.69066 0.12112 0 7.2951 0
0 51.394 3.371464 0 0.00011672 0 0.0018676 0 0.24116 0 0 11.841 0.69066
3.8586 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$PLWMAX= (0..7)
382.3078 100.8638 0 0 0 0 0
##$PQPHASE= 0
##$PQSCALE= 1
##$PR= 1
##$PRECHAN= (0..32)
-1 2 -1 0 1 3 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
-1 -1 -1 -1 -1 -1 -1 -1
##$PRGAIN= 0
##$PROBHD= <Z163572_0001 (CP TXO 900SA N/C-H-D-05 Z)>
##$PROBINPUTS= (0..15)
<13C> <15N> <1H> <2H> <> <> <> <> <> <> <> <> <> <> <>
##$PULPROG= <hetcor.jmod.pseudo3D.110518.rw>
##$PW= 0
##$PYNM= <>
##$ProjAngle= 0
##$QNP= 0
##$RD= 0
##$RECCHAN= (0..9)
0 3 1 0 0 0 0 0 0
##$RECPH= 0
##$RECPRE= (0..24)
-1 0 -1 2 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
##$RECPRFX= (0..32)
1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RECSEL= (0..24)
0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$RG= 101
##$RO= 0
##$RSEL= (0..24)
0 1 0 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$S= (0..7)
83 83 83 83 83 83 83 83
##$SELREC= (0..24)
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
##$SF01= 226.256560668938
##$SF02= 899.79089979
##$SF03= 899.79
##$SF04= 899.79
##$SF05= 899.79422902
##$SF06= 899.79422902
##$SF07= 899.79422902
##$SF08= 899.79422902
##$SOLVENT= <D20_salt>
##$SOLVOLD= <off>
##$SP= (0..63)
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120
120 120 120 120 120 120 120 120 120
##$SPECTR= 0
##$SPINCNT= 0
##$SPNAM= (0..63)
<> <Q5.1000> <Q3_surbop.1> <0.0> <Eburp2tr.1000> <Crp80comp.4> <Crp80,0.5,20.1>
<Sinc1.1000> <Crp80,0.5,20.1> <> <Crp80comp.4> <Crp80comp.4> <> <> <Eburp2.1000>
<> <> <> <0.0> <G4tr.256> <G4tr.256> <G4tr.256> <G4tr.256> <> <> <> <Gaus1_180r.1000>
<> <> <Q5tr.1000> <Q3_surbop.1> <Reburp.1000> <Q3.1000> <> <Q3_surbop.1>
<Q3_surbop.1> <Q5.1000> <> <> <> <Q3_surbop.1> <Crp80,0.5,20.1> <> <> <>
<> <> <> <> <> <> <> <> <> <> <> <> <> <> <> <> <> <> <>
##$SPOAL= (0..63)
0.5 1 0.5 0.5 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 1 0.5 0.5 0.5 0.5 0
```



##\$ZL3= 120  
##\$ZL4= 120  
##\$scaledByNS= no  
##\$scaledByRG= no  
##END=



```
##TITLE= Parameter file, TopSpin 4.0.4
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 18  $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= rvwillia
$$ 2018-11-13 17:01:25.245 -0500 rvwillia@br900
$$ /opt/nmrdata/rvwillia/13C-Me-Val-Robo1+Dy/7/acqu2s
$$ process /opt/topspin4.0.4/prog/mod/acqdataserver
##$ACQT0= 0
##$BF1= 899.789999996
##$FnILOOP= 1
##$FnMODE= 1
##$NUC1= <1H>
##$NusJSP= 0
##$NusT2= 1
##$NusTD= 16
##$O1= 4229.017
##$PULPROG= <hetcor.jmod.pseudo3D.110518.rw>
##$ProjAngle= 0
##$SF01= 899.794229013
##$SW= 9.99429143400936
##$SW_h= 8992.80575539568
##$TD= 16
##END=
```

```
##TITLE= Parameter file, TopSpin 4.0.4
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 33  $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= rvwillia
$$ 2018-11-14 16:24:07.289 -0500 rvwillia@br900
$$ /opt/nmrdata/rvwillia/13C-Me-Val-Robo1+Dy/7/acqu3s
$$ process /opt/topspin4.0.4/prog/mod/acqdataserver
##$ACQT0= 0
##$BF1= 899.789999996
##$FnILOOP= 1
##$FnMODE= 5
##$NUC1= <1H>
##$NusJSP= 0
##$NusT2= 1
##$NusTD= 32
##$O1= 4229.017
##$PULPROG= <hetcor.jmod.pseudo3D.110518.rw>
##$ProjAngle= 0
##$SF01= 899.794229013
##$SW= 3.00044602446501
##$SW_h= 2699.78401727862
##$TD= 32
##END=
```