Supplement of

Improved NMR transfer of magnetization from protons to half-integer spin quadrupolar nuclei at moderate and high magic-angle spinning frequencies

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Supporting Information

Table S1. Selected $R_{NN}^\nu \ |m\ |$ = 2 SQ hetero-nuclear dipolar recoupling for $\nu_R = 20$ kHz.

| $R$ | $R_{NN}^\nu$ | $\phi^\circ$ | $\nu_1/\nu_R$ | $\kappa$ | $\kappa/\parallel K_{(1,2)}^{DD_1\times DD_2} \parallel_2$ | $\kappa/\parallel K_{(1,2)}^{CSA\times CSA} \parallel_2$ | $\kappa/\parallel K_{(1,2)}^{\delta iso\times \delta iso} \parallel_2$ |
|-----|--------------|-------------|--------------|--------|---------------------------------|---------------------------------|---------------------------------|
| R22$^3_2$ | 57 | 5.5 | 0.178 | 162 | 7.12 | 17.58 |
| 180$^0_0$ | R28$^5_3$ | 51 | 4.67 | 0.176 | 156 | 5.08 | 18.29 |
| R18$^5_2$ | 50 | 4.5 | 0.175 | 140 | 7.20 | 18.49 |

Table S2. Selected $R_{NN}^\nu \ |m\ |$ = 2 SQ hetero-nuclear dipolar recoupling with $45^\circ \leq \phi \leq 135^\circ$ for $\nu_R = 62.5$ kHz.

| $R$ | $R_{NN}^\nu$ | $\phi^\circ$ | $\nu_1/\nu_R$ | $\kappa$ | $\kappa/\parallel K_{(1,2)}^{DD_1\times DD_2} \parallel_2$ | $\kappa/\parallel K_{(1,2)}^{CSA\times CSA} \parallel_2$ | $\kappa/\parallel K_{(1,2)}^{\delta iso\times \delta iso} \parallel_2$ |
|-----|--------------|-------------|--------------|--------|---------------------------------|---------------------------------|---------------------------------|
| 90$^0_0$240$^0_0$90$^0_0$ | R10$^3_4$ | 54 | 2.92 | 0.227 | 39.63 | 2.82 | 12.63 |
| R14$^5_6$ | 64.3 | 2.72 | 0.232 | 36.33 | 1.87 | 12.39 |
| R12$^4_5$ | 60 | 2.80 | 0.230 | 36.08 | 2.25 | 12.47 |
| R12$^8_7$ | 120 | 2.00 | 0.227 | 35.96 | 1.61 | 7.72 |
| 270$^0_0$90$^0_180$ | R16$^6_7$ | 67.5 | 2.28 | 0.150 | 17.96 | 1.85 | $3.50\times10^{10}$ |
| R16$^{10}_7$ | 112.5 | 2.28 | 0.150 | 17.96 | 1.85 | $3.50\times10^{10}$ |
| R14$^5_6$ | 64.3 | 2.33 | 0.150 | 15.90 | 2.33 | $3.58\times10^{10}$ |
| R14$^9_6$ | 115.7 | 2.33 | 0.150 | 15.90 | 2.15 | $3.58\times10^{10}$ |
| 90$^0_0$45$^0_0$45$^0_0$90$^0_45$ | R10$^3_4$ | 54 | 1.88 | 0.186 | 16.70 | 2.97 | 15.07 |
| R18$^5_7$ | 50 | 1.93 | 0.189 | 15.73 | 1.98 | 25.49 |
| R14$^5_6$ | 64.3 | 1.75 | 0.177 | 15.55 | 2.09 | 5.49 |
| R12$^4_5$ | 60 | 1.80 | 0.181 | 15.17 | 2.47 | 8.11 |
| 180$^0_0$ | R14$^5_6$ | 64.3 | 1.16 | 0.085 | 5.35 | 2.26 | 1.34 |
| R14$^9_6$ | 115.7 | 1.16 | 0.085 | 5.35 | 2.26 | 1.34 |
| R16$^6_7$ | 67.5 | 1.14 | 0.082 | 4.90 | 1.98 | 1.09 |
| R16$^{10}_7$ | 112.5 | 1.14 | 0.082 | 4.90 | 1.98 | 1.09 |

Table S3. Selected $R_{NN}^\nu \ |m\ |$ = 2 SQ hetero-nuclear dipolar recoupling built from single $\pi$ pulses with $20^\circ \leq \phi \leq 160^\circ$ and $\kappa \geq 0.15$ for $\nu_R = 62.5$ kHz.
| \( R \) | \( \text{RNN}^v_n \) | \( \phi/\degree \) | \( v_1/v_R \) | \( \kappa \) | \( \| K_{DD_1 \times DD_2}^{\text{D}} \|_2 \) | \( \| K_{CSA \times CSA}^{\text{D}} \|_2 \) | \( \| K_{\delta \text{iso} \times \delta \text{iso}}^{\text{D}} \|_2 \) |
|---|---|---|---|---|---|---|---|
| 180\(_0\) | R28\(_5^4\) | 101 | 4.66 | 0.131 | 63.17 | 16.48 | 9.31 |
| | R20\(_5^1\) | 99 | 4.66 | 0.131 | 60.68 | 16.59 | 14.45 |
| | R12\(_3^7\) | 79 | 4.66 | 0.131 | 45.52 | 15.76 | 13.60 |
| R28\(_7^3\) | 64 | 4.66 | 0.131 | 44.55 | 14.06 | 11.98 |
| | R20\(_5^9\) | 81 | 4.66 | 0.131 | 44.30 | 15.95 | 14.46 |
| | R12\(_3^5\) | 75 | 4.66 | 0.131 | 43.91 | 15.40 | 12.83 |
| SR4\(_1^2\) | 90 | 4.66 | 0.131 | 42.37 | 22.65 | 10.48 |
| 90\(_0\)-240\(_0\)-90\(_0\) | R28\(_7^7\) | 71 | 3 | 0.191 | 39.81 | 10.05 | 6.10 |
| | R20\(_5^8\) | 72 | 3 | 0.191 | 39.74 | 10.26 | 5.49 |
| | R8\(_2^3\) | 67.5 | 3 | 0.191 | 39.43 | 9.42 | 7.88 |
| | R8\(_2^3\) | 67.5 | 3 | 0.191 | 39.43 | 9.42 | 7.88 |
| R24\(_5^4\) | 75 | 3 | 0.191 | 39.32 | 10.66 | 4.22 |
| | R28\(_7^7\) | 64.3 | 3 | 0.191 | 38.82 | 8.65 | 10.13 |
| | R12\(_3^5\) | 75 | 3 | 0.191 | 38.33 | 10.66 | 4.22 |
| SR4\(_1^2\) | 90 | 3 | 0.191 | 19.95 | 19.48 | 1.33 |
| 90\(_0\)-45\(_0\)-90\(_0\)-45 | R24\(_5^4\) | 75 | 3 | 0.191 | 39.32 | 10.66 | 4.22 |
| | R28\(_7^7\) | 64.3 | 3 | 0.191 | 38.82 | 8.65 | 10.13 |
| | R12\(_3^5\) | 75 | 3 | 0.191 | 38.33 | 10.66 | 4.22 |
| SR4\(_1^2\) | 90 | 3 | 0.191 | 19.95 | 19.48 | 1.33 |
| 270\(_0\)-90\(_180\) | R24\(_5^1\) | 82.5 | 4 | 0.212 | 33.12 | 25.46 | 8.67 \times 10^{10} |
| | R20\(_5^9\) | 81 | 4 | 0.212 | 31.85 | 25.19 | 8.67 \times 10^{10} |
| | R20\(_5^3\) | 99 | 4 | 0.212 | 31.85 | 25.19 | 8.67 \times 10^{10} |
| R16\(_4^7\) | 78.8 | 4 | 0.212 | 28.56 | 24.69 | 8.67 \times 10^{10} |
| | R16\(_4^9\) | 101.2 | 4 | 0.212 | 28.56 | 24.69 | 8.67 \times 10^{10} |
| | R12\(_3^5\) | 75 | 4 | 0.212 | 20.84 | 23.58 | 8.67 \times 10^{10} |

Table S4. Selected \( \text{RNN}^v_n \) \( |m| = 2 \) two-spin order hetero-nuclear dipolar recoupling.
Figure S1: $^1$H MAS spectrum of AlPO$_4$-14 acquired at $B_0 = 18.8$ T and $\nu_R = 20$ kHz by averaging 16 transients separated by a recycle interval of 1 s, using the DEPTH pulse sequence for probe background suppression, with $\nu_1 \approx 208$ kHz (Cory and Ritchey, 1988).
Figure S2: $^{27}$AlO$_4$ signal of AlPO$_4$-14 at $\nu_R = 20$ kHz as function of $\nu_1$ or $\nu_{1,\text{max}}$ of the recoupling for PRESTO-R22$^2_2(180\theta)$ and -R18$^5_2(180\theta)$ as well as RINEPT-CWc-SR4$^2_1$(tt), -SR4$^2_1(270\theta90\nu_{180})$ and -R12$^5_3(270\nu_{90180})$. For each curve, $\tau$ was fixed to its optimum value given in Table 2.

Figure S3: $^{27}$AlO$_4$ signal of AlPO$_4$-14 at $\nu_R = 20$ kHz as function of offset of the recoupling for PRESTO-R22$^7_2(180\theta)$ and -R18$^5_2(180\theta)$ as well as RINEPT-CWc-SR4$^2_1$(tt), -SR4$^2_1(270\theta90\nu_{180})$ and -R12$^5_3(270\nu_{90180})$. For each curve, $\tau$ and $\nu_1$ or $\nu_{1,\text{max}}$ were fixed to their optimum values given in Table 2.
Figure S4: $^{27}$AlO$_4$ signal of AlPO$_4$-14 at $\nu_R = 62.5$ kHz as function of $\nu_1$ or $\nu_{1,\text{max}}$ of the recoupling for PRESTO-R$16_6^5(270_90_{180})$ and -R$14_6^5(270_90_{180})$ as well as RINEPT-CWc-SR$4_1^2$ (tt), -SR$4_1^2$ (270_90_{180}) and -R$12_3^5$ (270_90_{180}). For each curve, $\tau$ was fixed to its optimum value given in Table 4.

Figure S5: $^{27}$AlO$_4$ signal of AlPO$_4$-14 at $\nu_R = 62.5$ kHz as function of offset of the recoupling for PRESTO-R$16_6^5(270_90_{180})$ and -R$14_6^5(270_90_{180})$ as well as RINEPT-CWc-SR$4_1^2$ (tt), -SR$4_1^2$ (270_90_{180}) and -R$12_3^5$ (270_90_{180}). For each curve, $\tau$ and $\nu_1$ or $\nu_{1,\text{max}}$ were fixed to their optimum values given in Table 4.
Figure S6: Skyline projections along F₂ of ¹H-²⁷Al HETCOR 2D spectra of AlPO₄-14 recorded with RINEPT-CWC-SR₄₂ (270°, 90°, 180°), SR₄₂(tt), SR₄₂(180°, 90°, 180°) and PRESTO-R16₆ (270°, 90°, 180°) transfers. All 2D spectra were acquired using NUS 25% in 72 min.

Figure S7: Skyline projections along F₁ of ¹H-²⁷Al HETCOR 2D spectra of AlPO₄-14 recorded with RINEPT-CWC-SR₄₁ (270°, 90°, 180°), SR₄₁(tt), SR₄₁(180°, 90°, 180°) and PRESTO-R16₆ (270°, 90°, 180°) transfers. All 2D spectra were acquired using NUS 25% in 72 min.
Table S5. Distances between the different hydrogen atoms and their closest Al neighbours in the structure of isopropylamine templated AlPO₄-14 determined from X-ray diffraction. (Broach et al., 2003) The H and Al atoms are numbered according to the cif file.

|       |       | r_{HAI}/Å |
|-------|-------|-----------|
| H1 (OH) | Al4O₆ | 2.496 |
|     | Al4O₆ | 2.499 |
|     | Al1O₅ | 2.503 |
|     | Al2O₄ | 4.299 |
| H2 (NH₃) | Al4O₆ | 3.069 |
|     | Al2O₄ | 3.779 |
| H3 (NH₃) | Al3O₄ | 3.778 |
|     | Al4O₆ | 3.960 |
| H4 (NH₃) | Al2O₄ | 3.479 |
|     | Al1O₅ | 3.801 |
| H5 (CH) | Al2O₄ | 3.737 |
|     | Al1O₅ | 4.850 |
| H6 (CH₃) | Al1O₅ | 3.655 |
|     | Al3O₄ | 4.594 |
| H7 (CH₃) | Al3O₄ | 4.082 |
|     | Al1O₅ | 4.320 |
| H8 (CH₃) | Al2O₄ | 3.772 |
|     | Al3O₄ | 4.651 |
| H9 (CH₃) | Al4O₆ | 3.888 |
|     | Al3O₄ | 4.124 |
| H10 (CH₃) | Al4O₆ | 3.509 |
|     | Al3O₄ | 4.502 |
| H11 (CH₃) | Al4O₆ | 3.970 |
|     | Al3O₄ | 4.048 |

Broach, R. W., Wilson, S. T., Kirchner, R. M.: Corrected crystallographic tables and figure for as-synthesized AlPO₄-14, Microporous and Mesoporous Materials, 57, 211–214, https://doi.org/10.1016/S1387-1811(02)00563-2, 2003.
Pulse sequence for D-RINEPT using $SR\alpha_1^2$ (270°90°) or $R_1\alpha_3^5$ (270°90°) recouplings

; INEPT for non-selective polarization transfer
; with decoupling during acquisition
; made of 2 pulses
; different recoupling sequences and composite pulses available

; modified by Julien Trébosc and Jennifer Gómez (2020)
; AVANCE NEO

:d0 initial t1 evolution time (=0)
:d6 probe dead time (should be D6=DE)
:d7 RF offset delay
:d5 Delay after last recoupling for Tr/2
:d8 Delay after last recoupling for Tr/4
:pl1 p1 and p2 power level
:pl12 Heteronuclear dipolar decoupling
:pl19 Presat pulse
:pl20 Presat pulse
:pl21 p3 and p4 power level
:pl22 initial spin lock
:pl33 CW23 decoupling
:pl43 CW45 decoupling
:pl44 CW67 decoupling
:pl11 dipolar recoupling power (sr4/sfam)
:spnam5 dipolar recoupling shape pulse
:pl16 : requested recoupling time
:pl17 : actual recoupling time
:l11 sr4/sfam repetition
:cnst30: Tanh/tan offset
:cnst31: spinning speed in Hz
:cnst3: Tanh/tan shape pulse step (ns)
:p1 90 degree pulse for X
:p2 180 degree pulse for X
:p3 90 degree pulse for 1H
:p4 180 degree pulse for 1H
:p19 presat pulse for 1H
:p20 presat pulse for X
:p22 initial spin lock for Tr/2
:p23 initial spin lock for Tr/4
:p33 CW45 decoupling for Tr/2
:p34 CW45 decoupling for Tr/4
:p43 CW23 decoupling for Tr/2
:p44 CW67 decoupling for Tr/2
:: CW23 decoupling for Tr/4
:: CW67 decoupling for Tr/4
:: d1: relaxation delay; 1-5 * T1
:: NS: 16 * n, total number of scans: NS * TD0
:: DS: 16
:: cpd1: decoupling during R3
:: cpdprg1: decoupling during R3
:: cpd2: decoupling during AQ and t1
:: cpdprg2: decoupling during AQ and t1
:: cpd3: decoupling during AQ
:: cpdprg3: decoupling during AQ

#include <Avance.incl>

; storeVC option to store VClst used when popting MAS
#ifndef storeVC
#define VCstored vclab, 1u \n lo to vclab times c
#else
#define VCstored
#endif

#include "presat.incl"

ifndef PRESATf2
#undef PRESAT2
#define PRESAT2(f2)
#endif

ifndef PRESATf1
#undef PRESAT1
#define PRESAT1(f1)
#endif

ifndef decF2
#define decF2off do:f2
#define decF2aqon cpds2:f2
#else
#define decF2aqon
#define decF2off
#endif

define delay RF
define delay dummy
```
#define phaseRN (360) \{\{90 270 270 90\}*2\}^180^240
  "p6=0.25s/cnst31"
  "p7=p6*3/4.0" ; p270 deg
  "p8=p6/4.0"  ; p90 deg
 ; we have p6 = p7 + p8
 ;"l11=trunc((p16/p6)/4+0.5)" ; +0.5 will round to nearest integer
  "p17=2*p6*2*l11"
  "RF=250e3/p8"
  "dummy=RF+p17"
#endif

#define phaseRN (360) 75 255 285 105
  "p6=0.25s/cnst31"
  "p7=p6*3/4.0" ; p270 deg
  "p8=p6/4.0"  ; p90 deg
 ; we have p6 = p7 + p8
 ;"l11=trunc((p16/p6)/4+0.5)" ; +0.5 will round to nearest integer
  "p17=2*p6*2*l11"
  "RF=250e3/p8"
  "dummy=RF+p17"
#endif

;d24=p3
  "p2=p1*2"
  "p4=p3*2"
 ;"d6=de"
  "p22=0.5s/(cnst31)-p3/2.0"
  "p23=0.25s/(cnst31)-p3/2.0"
  "d5=0.5s/(cnst31)-d6"
  "d8=0.25s/(cnst31)-d6"
  "p33=0.5s/(cnst31)-p3"
  "p34=0.25s/(cnst31)-p3-p4"
  "p44=0.5s/(cnst31)-p4/2.0"
  "p46=0.25s/(cnst31)-p4/2.0"
  "p55=0.5s/(cnst31)-d6"
  "p43=0.5s/(cnst31)-p4/2.0-p3"
  "p45=0.25s/(cnst31)-p4/2.0"
  "d7=0.00000005s"
  "plw43=plw33"
  "plw44=plw33"

"in0=inf1"

#define delay showInAsed
  "showInAsed=cnst3+dummy"
```
l ze
VCstored
"showInAsed=cnst3+dummy"

2 30m decF2off
PRESAT2(f2)
d1 rpp16 rpp17 rpp14 rpp15 ; not necessary to use different phases and reset but...
PRESAT1(f1)
(10u pl21):f2 (10u pl1 ph2):f1
(p3 ph1):f2

#ifndef _iSL
if "l11 % 2 == 0"
{
    (p22 pl22 ph27):f2
}
else
{
    (p23 pl22 ph27):f2
}
#endif

d0

sr4_1, (p7 pl11 ph16^):f2
(p8 pl11 ph16^):f2
(p7 pl11 ph16^):f2
(p8 pl11 ph16^):f2
lo to sr4_1 times l11

if "l11 % 2 == 0"
{
    (center (p3 pl21 ph18 p43 pl43 ph21 p4 pl21 ph2 p43 pl43 ph22 p3 pl21 ph18):f2 (p2 ph11):f1 )
}
else
{
    (center (p45 pl43 ph18 p4 pl21 ph2 p45 pl43 ph18):f2 (p2 ph11):f1 )
}

sr4_2, (p7 pl11 ph17^):f2
(p8 pl11 ph17^):f2
(p7 pl11 ph17^):f2
(p8 pl11 ph17^):f2
lo to sr4_2 times l11

if "l11%2 == 0"
{
    (center (p3 pl21 ph18 p33 pl33 ph23 p33 pl33 ph24 p3 pl21 ph3):f2 (p1 ph12):f1 )
}
} else
{ (center (p4 pl21 ph5 p3 pl21 ph3 p34 pl33 ph21 p34 pl33 ph22 p4 pl21 ph5 p3 pl21 ph3):f2 (p1 ph12):f1 )
}

sr4_3, (p7 pl11 ph15^):f2
  (p8 pl11 ph15^):f2
  (p7 pl11 ph15^):f2
  (p8 pl11 ph15^):f2
lo to sr4_3 times l11

if "l11%2 == 0"
{ (center (p44 pl44 ph25 p4 pl21 ph2 p44 pl44 ph26):f2 (p2 ph13):f1 )
}
else
{ (center (p46 pl44 ph25 p4 pl21 ph2 p46 pl44 ph26):f2 (p2 ph13):f1 )
}

sr4_4, (p7 pl11 ph14^):f2
  (p8 pl11 ph14^):f2
  (p7 pl11 ph14^):f2
  (p8 pl11 ph14^):f2
lo to sr4_4 times l11

if "l11%2 == 0"
{ d5 decF2aqon
}
else
{ d8 decF2aqon
}
go=2 ph31
10u decF2off
30m mc #0 to 2 F1PH(ip1,id0)

HaltAQ, 1m

exit

ph0=0
ph2=0

ph3=0
ph4=0
ph5= (360) 45
ph6=0
ph7=0
ph10=0
ph11={\{0\}*2}^2
ph12={\{0\}*4}^2
ph13={\{0\}*8}^2^1^3
ph18=1
ph21=0
ph22=2
ph23=0
ph24=2
ph25=0
ph26=2
ph27=0 2
ph28=0
ph29=3
ph16= phaseRN
ph17= phaseRN
#ifdef opt1D
ph1=1 3 0 2
ph31=3 1 2 0
#else
ph1=1 3
ph31={\{1 3\}^0}^2^0^2^2
#endif
presatPH

SIMPSON input file for $D$-RINEPT-CW$_c$-SR$4^2_1$(tt)

spinsys {
  channels  1H 13C
  nuclei  1H 13C 1H 1H 1H
  # single pair
  shift  1 0 6000 0 0 30 0
  dipole  1 2 -2575 0 0 0
  # 2 1H
  shift  3 0 6000 0 0 30 0
  dipole  3 2 0 0 109 0
  dipole  1 3 -7000 0 109 0
  # 3 1H
  shift  4 0 6000 0 0 30 0
  dipole  4 2 0 0 109 120
  dipole  1 4 -7000 0 109 120
  dipole  3 4 -7000 0 90 30
  # 4 1H
  shift  5 0 6000 0 0 30 0
  dipole  5 2 0 0 109 240
  dipole  1 5 -7000 0 109 240
\begin{verbatim}
dipole 3 5 -7000 0 90 90
dipole 4 5 -7000 0 90 330
}

par {
    proton_frequency 400e6
    spin_rate 12500
    sw spin_rate/2.0
    np 30
    crystal_file rep66
    gamma_angles 7
    start_operator I1z
    detect_operator I2p
    verbose 1101
    variable HRF 100000
    variable DRF 92000
    variable CRF 100000
    variable RFmax spin_rate*11
    variable offmax 200000
    variable I 1.0/2.0
}

proc gen_tanhtan_shape {pulse_length steps offmax xi K} {
    # generate a tanhtan shape with given:
    # pulse_length : length of pulse in us
    # steps : number of steps defining the shape
    # offset : maximum frequency offset of tanhtan sweep
    # xi : tanhtan xi parameter
    # K : tanhtan kappa parameter
    set nhalf [expr $steps/2]
    set amp_list [list ]
    set phase_list [list ]
    for {set i 0} {$i < $steps} {incr i} {
        set x [expr 1.0*$i/(1.0*$steps)]
        if {$i<$nhalf} {
            lappend amp_list [expr tanh(2*$xi*$x)]
        } else {
            lappend amp_list [expr tanh(2*$xi*(1-$x))]
        }
        lappend phase_list [expr -360*$offmax*$pulse_length*(1e-6)*log(abs(cos($K*(1-2*$x))))/(2*tan($K)*$K)]
    }
    set Tinc [expr 1.0*$pulse_length/$steps]
    return [list $amp_list $phase_list $Tinc]
}

proc tanhtan_pulse {shape RF phase} {
    # generate simpson pulse following shape argument containing amplitude and phase lists
    # shape: as generated by gen_tanhtan_shape procedure
    # RF : global maximum RFfield of shape
    # phase : global phase of shape
\end{verbatim}
```
set amp_list [lindex $shape 0]
set phase_list [lindex $shape 1]
set Tinc [lindex $shape 2]
foreach amp $amp_list phi $phase_list {
    pulse $Tinc [expr $amp*$RF] [expr $phase+$phi] 0 0
}
proc pulseq {} {
    global par
    maxdt 6.0
    set H90  [expr 0.25e6/$par(HRF)]
    set H180 [expr 0.50e6/$par(HRF)]
    set C90  [expr 0.25e6/$par(CRF)]
    set C180 [expr 0.50e6/$par(CRF)]
    set Taur [expr 1.0e6/$par(spin_rate)]
    set Td90  [expr 0.5e6/$par(spin_rate)-$H90/2]
    set Td180 [expr 0.5e6/$par(spin_rate)-$H180/2]
    # RN_n^nu parameters
    set N 4.
    set nu 2.
    set n 1.
    set phi [expr 180*$nu/$N]
    set S90 [expr 0.25e6/$par(RFmax)]
    set S180 [expr 0.50e6/$par(RFmax)]
    set n 100
    set Tp [expr 0.25*$Taur]
    set Tpd [expr 0.25*$Taur]
    set xi 10.0
    set K   atan(20)
    set pi   [expr atan(1)*4]
    set shape [gen_tanhtan_shape $Tp $n $par(offmax) $xi $K ]
    set ph1 0
    set ph2 120
    set ph3 240
    # SR4 using tanhtan inversion
    # full block with supercycling
    set superCycling {0 180 120 300 240 60}
    reset
    foreach ph1 $superCycling {
        reset
        for {set s 0 } {$s<$N/2} {incr s } {
            delay [expr $Tpd/2-$Tp/2]
        }
    }
```
tanhtan_pulse $shape $par(RFmax) [expr $php+$ph1]
  delay [expr $Tpd/2-$Tp/2]
  delay [expr $Tpd/2-$Tp/2]
tanhtan_pulse $shape $par(RFmax) [expr -$php+$ph1]
  delay [expr $Tpd/2-$Tp/2]
}
store $ph1
}
reset [expr -$H90]
pulse $H90 $par(HRF) 90 0 0
  # pulse $Td90 $par(DRF) 0 0 0
  store 19
reset
pulse $Td180 $par(DRF) 0 0 0
pulse $H180 $par(HRF) 0 $par(CRF) 0
pulse $Td180 $par(DRF) 180 0 0
store 20
reset
pulse $Td90 $par(DRF) 0 0 0
pulse $H90 $par(HRF) 0 $par(CRF) 0
pulse $Td90 $par(DRF) 180 0 0
store 20
reset
pulse $Td180 $par(DRF) 0 0 0
pulse $H180 $par(HRF) 0 $par(CRF) 0
pulse $Td180 $par(DRF) 180 0 0
store 22
reset
  # prop [expr (0%[llength $superCycling])*[lindex $superCycling 1]]
  prop [lindex $superCycling 0]
  store 10
for {set i 0} {$i < $par(np)} {incr i} {
  #reset
  reset [expr -$H90]
  # pulseid $H90 $par(HRF) 90 0 0
  prop 19
  prop 10
  prop 20
  prop 21
  prop 10
  prop 22
  prop 10
}
pulse [expr $Taur/2.0] $par(DRF) 0 0 0
acq
reset
prop 10
# puts [expr (($i+1)%[llength $superCycling])*[lindex $superCycling 1]]
# prop [expr (($i+1)%[llength $superCycling])*[lindex $superCycling 1]]
prop [lindex $superCycling [expr (($i+1)%6)]]
store 10
}
}
proc main {} {
  global par
  set FileRe [open "$par(name)-Re.res" w]
  set FileIm [open "$par(name)-Im.res" w]
  set FileAbs [open "$par(name)-Abs.res" w]
  set f [fsimpson]
  set c 0
  for {set i 1} {$i <= $par(np)} {incr i} {
    incr c
    set Sr [findex $f $c -re]
    set Si [findex $f $c -im]
    puts $FileRe "[expr 1.0e3*$i/$par(sw)] [expr $Sr]"
    puts $FileIm "[expr 1.0e3*$i/$par(sw)] [expr $Si]"
    puts $FileAbs "[expr 1.0e3*$i/$par(sw)] [expr sqrt($Sr**2+$Si**2)]"
  }
  funload $f
  close $FileRe
  close $FileIm
  close $FileAbs
}