Q-SwitchTM accessory

NMR Probes with Switchable Quality Factor



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Warning

THE Q-SWITCHTM ACCESSORY OPERATES WITH HIGH VOLTAGES. ALWAYS DISCONNECT THE POWER CORD FROM THE RF CHANNEL SELECTOR UNIT BEFORE OPENING THE PROBE, THE RF CHANNEL SELECTOR OR THE RF DUPLEXER

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Table of Contents

1	Introduction
2	Reduction of Radiation Damping
3	The Q-Switch TM accessory
4	Experiments with the Q-Switch TM probe
4.	1 Experimental Set-Up
4.	2 Inversion Recovery T1-measurements
4.	3 Q-Switching during free precession delays
4.4	4 Q-Switching during acquisition
4.	5 Selective excitation and Q-Switching
5	References
6	Appendix
6.	1 Definitions for Q-Switching 19
6.	2 Inversion Recovery T1 measurements
6.	3 Noesy with Q-Switching during evolution
6.4	4 Q-Switched Selective Pulse

1 Introduction

The mutual coupling between a strong NMR signal and the receiver coil leads to a phenomenon called radiation damping¹. The transverse magnetization component of an abundant spin species, such as that of a protonated solvent, induces a relatively large current in the coil. In turn this current generates a weak rotating magnetic field, at the exact frequency of the resonance from which it originates and as a result the magnetization is tilted back towards its equilibrium position.

Although, as pointed out by Abragam², the term radiation damping is not correct since the length of the magnetization vector is unchanged, this mechanism does result in a damping of the observable free induction decay by reducing the time the magnetization spends in the transverse plane. This in turn leads to a broadening of the resonance line. Figure 1 shows two proton free induction decays of water, observed after excitation with a 90° pulse and a 180° pulse, respectively, which demonstrate the fast decay of the resonance signal due to radiation damping and the echo-type response due to the magnetization being tilted back from anti-parallel to parallel to the main magnetic field after a 180° pulse.

Although radiation damping is not a new phenomenon, its effects in high resolution NMR spectroscopy have gained importance with the availability of higher magnetic field strengths and of probes with increased sensitivity (higher quality factor Q).

Radiation damping causes degeneration of solvent suppression and selective excitation techniques³ and is responsible for non-exponential relaxation processes⁴ and harmonic peaks in high resolution experiments⁵. Especially in NMR of biomolecules in aqueous solution the strong proton magnetization of the bulk water leads to a line broadening of not only the water resonance but also of resonances of spins that exchange with water.



Figure 1 *Proton free induction decays of water obtained after excitation with a 90 degree pulse (top) and a 180 degree pulse (bottom), demonstrating the effects of radiation damping.*

2 Reduction of Radiation Damping

The rate of change of the magnetization vector due to radiation damping can be characterized by a time constant τ_d which depends on the amount of magnetization, the gyromagnetic constant γ of the spins and the quality factor Q of the probe^{2,3}:

(1)
$$\tau_d^{-1} = 2\pi Q \eta \gamma M_0$$

in which M_0 is the equilibrium magnetization and η is the filling factor of the coil.

Radiation damping can sometimes be avoided by saturating the strong resonance prior to the NMR measurement, but this approach is often not desirable since it leads to attenuation of the resonance intensities of exchanging protons. Other attempts to reduce or eliminate the radiation damping phenomena (lengthen τ_d) are aimed at reducing the mutual coupling between the magnetization and the RF coil and can be divided into different strategies.

The first and most commonly employed strategy is to detune the probe circuit², thereby effectively reducing the quality factor Q of the probe and thus reducing the rate at which the magnetization vector is tilted back to the direction of the main magnetic field (eq.1). A disadvantage of this approach is a loss in signal intensity; the induced voltage in the coil, and thus the sensitivity, is proportional to the Q of the resonance circuit.

A second strategy is to neutralize the voltage in the receiver coil, induced by the strong NMR signal. This cancellation prevents the occurrence of a sizable current in the RF coil and thus eliminates radiation damping. The neutralization of the induced voltage is achieved via an electronic feedback circuit and this approach has the benefit of preserving the signal to noise ratio, provided that the feedback loop is noise free. Two experimental implementations of electronic feedback circuits to cancel radiation damping have been proposed by Broekart and Jeener⁶ and by Louis-Joseph et al.⁷ Both implementations are ingenious but are quite demanding on hardware and do cause a loss in signal intensity from the insertion of additional elements in the probereceiver circuit.

A different approach is related to spectroscopy with radio frequency gradients. In RF GRASPTM a probe is employed which has a dual coil design⁸, one coil to generate the homogeneous RF magnetic field and a second coil which generates an RF gradient field with a quadrupolar geometry. The coils are isolated through an active switching mechanism. Due to the different spatial geometries of the RF fields generated by these coils, a signal excited with one coil will have the wrong symmetry to induce a current in the other coil; the mutual coupling of the spins and the RF coil is zero. So by exciting with one coil and then switching to the other coil, radiation damping is effectively eliminated⁹. This approach allows the elimination of radiation damping during time intervals in the pulse sequence outside the acquisition window.

Another strategy of dealing with radiation damping involves the use of B_0 gradients. If transverse magnetization is subjected to a gradient field, the magnetization is dephased, and can therefore not induce a coherent current in the receiver coil, thus eliminating radiation damping. The use of gradients has been proposed¹⁰ as a means to avoid radiation damping effects in for instance the t₁-

evolution time of a 2D experiment, by using a dephasing gradient during the first half of the evolution time and a rephasing gradient during the second half. The gradients should be strong enough to quench radiation damping, but weak enough to minimize losses in signal intensity due to molecular diffusion¹¹. A similar approach involving the use of B_1 gradients has been demonstrated by Otting¹².



Figure 2 2D proton spectra of water, obtained with a NOESY sequence without (left) and with (right) Q-Switching during t_1 .

The approach employed in Bruker's line of **Q-Switch**TM probes is to actively switch the quality factor of the probe^{13,14}. The Q of the resonant circuit can be rapidly (< 2 μ s) switched back and forth between a high value, in the regular mode of operation, and an essentially zero Q mode. In the low Q mode radiation damping is effectively eliminated, while the full sensitivity and RF efficiencies are preserved by switching to high Q during acquisition and RF pulses. The simplicity and effectiveness of this approach is shown in Figure 2. In these spectra a water proton resonance is shown, obtained with a simple exchange experiment (no water suppression). Without Q-Switching (left spectrum) the linewidth in both dimensions is determined by radiation damping. In a second experiment the probe is switched to the low Q mode during the t₁-evolution time, which eliminates the linebroadening due to radiation damping and the corresponding spectrum (right) displays the natural linewidth of water in the first frequency dimension.

3 The Q-SwitchTM accessory

The **Q-SwitchTM** accessory consists of a **Q-SwitchTM** probe and a stand-alone switching unit, called the RF Channel SelectorTM.

Although there are no design limitations as to what type of probe is equipped with Q-switching, the advantages of a switchable quality factor are clearly most pronounced at high frequencies. The radiation damping rate, $\tau_d^{-1}=2\pi Q\eta\gamma M_0$, increases with higher magnetic field strength and with filling factor and is largest for proton magnetization. Q-switching is therefore suggested for proton dedicated or inverse detection probes at frequencies of 500 MHz and up.

The switching of the quality factor of the probe is achieved via an active switching mechanism, driven by the RF Channel SelectorTM. Switching is controlled from the pulse program via a control signal. By convention **NMRword8 bit 7** is used to switch the probe between the gradient mode and the homogeneous mode, via the commands **HIGHQ** and **LOWQ** (see also the appendix and the experimental section). Typically less than 2μ s is needed for switching. Switching the probe to its low Q state affects the tuning of the lock channel. For short periods of

Switching the probe to its low Q state affects the tuning of the lock channel. For short periods of low Q this will not have an effect on the experiment. For longer durations of the low Q state this may cause the loss of the lock signal and in those experiments we suggest the use of the lockhold feature of the BSMS, which is located on the front panel of the Lock Control Board (LCB).

4 Experiments with the Q-SwitchTM probe

In the following sector the experimental set-up for the **Q-SwitchTM** accessory is discussed and examples are given of experiments in which Q-switching is applied to eliminate the effects of radiation damping. The pulse programs for some of these experiments are given in the appendix.

4.1 Experimental Set-Up

The set-up of the Q-SwitchTM accessory is shown schematically in Figure 3. Please read the instruction manual for the RF Channel SelectorTM unit.

The **Q-SwitchTM** accessory consist of a **Q-SwitchTM** probe and an RF Channel Selector unit. The RF Channel Selector unit operates on 220V, which originates from the console. A burndy cable connects the probe with the RF Channel Selector via the connector labeled *PROBE*. For normal operation (i.e. high Q) the probe has to be connected to RF Channel Selector, which has to be on and the spectrometer type has to be selected on the front panel (*AMX/DMX*). The high Q state is indicated on the front panel of the RF Channel Selector (*CH1 is lit*). For testing purposes the probe can be manually switched between the high Q mode (*CH1 HIGH*) and the low Q mode (*CH1 LOW*).

Switching of the probe between the high Q and low Q modes is performed via a TTL signal, which is connected to the RF Channel Selector input *TTL IN*. On Avance-series instruments the switching is controlled from the pulse program via **NMRword8 bit 7**. The output of this control word can be found on the Timing Control Unit (**TCU**, **connector T3**, **pin T**). The following definitions are used:

#define HIGHQ setnmr8^7 and

#define LOWQ setnmr8|7

These definitions are included in each pulse program or alternatively can be added to the *Avance.incl* file (see appendix).

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Q-SwitchTM



Figure 3 Set-up of the Q-SwitchTM accessory.

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4.2 Inversion Recovery T₁-measurements



Figure 4 *Pulse sequence of the inversion recovery experiment, with Q-Switching during the recovery delay* τ *.*

A clear manifestation of radiation damping is found in experiments in which a large magnetization is stored anti-parallel to the main magnetic field direction. Due to radiation damping this magnetization is rapidly rotated back to the positive z-axis. For instance an inversion recovery T_1 measurement (Figure 4) on water in a probe with a high Q does not yield a single exponential decay⁴. An example is shown in Figure 5 where the integrated proton intensities of a 1:1 mixture of H₂O and D₂O are plotted as a function of the recovery time τ in an inversion recovery experiment¹³. After the 180 degree pulse, radiation damping causes the magnetization to rotate back to the positive z axis in a time much shorter than the T_1 relaxation time of the water protons. By switching the Q low during the recovery interval τ radiation damping is prevented and the rate of return of the magnetization to parallel to the main magnetic field is determined by the T_1 relaxation time. The data in Figure 5 display the expected single

exponential recovery from which the T_1 can be correctly obtained¹³.



Figure 5 600 MHz proton inversion recovery data from an 1:1 mixture of H_2O and D_2O . Circles represent data obtained with a high Q during the recovery delay, while the squares are data obtained with the Q of the probe switched to low during τ .

4.3 Q-Switching during free precession delays



Figure 6 Pulse scheme for a NOESY experiment with Q-switching during t_1 . Solvent suppression is achieved via a jump-return sequence prior to acquisition.

Radiation damping results in a linebroadening of not only the strong resonance but also of resonances that exchange with e.g. the solvent. In multi-dimensional experiments this leads to a loss in resolution and sensitivity. For instance in NOESY experiments (Figure 6) the intermolecular cross peaks between water and proteins or the cross peaks between hydration water and solute protons suffer from substantial linebroadening in the frequency domain of the water resonance. This is illustrated in Figure 7A which shows the cross peaks between the water signal at 4.7 ppm in F_1 and the NH and aromatic CH resonances of lysozyme in the F_2 dimension¹³.

The linebroadening due to radiation damping during free precession delays can be eliminated by switching the probe to low Q during these time intervals. The spectrum shown in Figure 7B is obtained from the same lysozyme sample as in A but with the Q of the probe set to low during the t_1 evolution time. This results in significant narrower protein-water cross peaks in the F_1 domain and a consequent gain in both sensitivity and resolution.

In this particular experiment¹³ water is suppressed just prior to acquisition via a 1,-1 sequence. The Q of the probe is high during the 150 ms mixing time, in which the water magnetization is aligned along the positive z-axis by radiation damping. This results in an excellent water suppression by the jump-return sequence, which is designed for starting from positive z-magnetization.

The NOESY experiment with Q-Switching during the evolution time¹³ exemplifies the benefits of Q-Switching to the study of water-protein interactions. Extension to other techniques, such as ROESY, TOCSY and other multi-dimensional experiments and variations on this NOESY experiment, as well as Q-Switching during other delays in the pulse sequence are straightforward and easy to implement.



Figure 7 Region of a 600 MHz proton NOESY spectra of 8 mM lysozyme in 90% $H_2O/10\%$ D_2O , showing cross peaks between water at 4.7 ppm and the low field signals of lysozyme. The Q of the probe was high throughout the whole experiment for the spectrum shown in A, while the Q was low during the t_1 evolution time for the spectrum in B.

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Figure 8 Pulse scheme for Q-Switching during acquisition.

The rapid switching capabilities of the **Q-Switch**TM accessory allows the suppression of radiation damping during data acquisition¹⁴. The Q is switched low during the time between taking datapoints and high when the datapoints are sampled (see Figure 8). In Figure 9 the proton free induction decays of a water resonance are depicted, obtained after a 90° and 180° pulse, respectively, and with Q-switching during data acquisition. In comparing these decays with those in Figure1 the reduction of the effect of radiation damping is apparent.



Figure 9 *Proton free induction decays of water obtained after excitation with a 90 degree pulse (top) and a 180 degree pulse (bottom), acquired with Q-Switching during acquisition.*

In the case of rapid switching between a high and low Q mode it is possible to define an effective, time-averaged Q value of the resonant circuit, which is a function of the off ratio of the Q-switching:

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(2)
$$Q_{eff}(t_{low}) = (1 - t_{low}/t_s)Q_{high}$$

where Q_{eff} is the effective quality factor during acquisition, Q_{high} is the quality factor of the probe operating in the regular mode, t_{low} is the time interval in which the Q is switched low and t_s is the sampling interval. The lowering of the effective Q during data acquisition reduces the rate constant for radiation damping and thus leads to a narrowing of the resonance line. In Figure 10 the linewidth at half height Δ_{HH} of a water resonance is plotted as a function of the off ratio t_{low}/t_s

¹⁴. A maximum off ratio of 0.85 is used in order to allow sufficient time for data sampling. Under these conditions line narrowing of a factor three is accomplished.



Figure 10 Linewidth at half height (Δ_{HH}) of a water resonance, obtained with Q-Switching during data acquisition, plotted as a function of the off-ratio t_{low}/t_s .

Figure 11 shows proton spectra of a 2 mM sucrose sample in 90% H_2O , acquired after a single excitation pulse. The spectra depicted in Figures 11A and the expansion 11C, are acquired in the regular high Q mode whereas Q-switching was applied during the acquisition of the spectra in Figures 11B and D with a off ratio of 0.85, resulting in a line narrowing factor of three for the water resonance and an improved resolution in the water region.

The suppression of radiation damping during acquisition is only needed if the spectrum is acquired in the presence of the full solvent signal. In most experiments the solvent signal is suppressed prior to data acquisition thereby eliminating radiation damping altogether. Q-switching during data acquisition leads to a loss in signal to noise, which is caused by the transients induced in the analog filters in the receiver, due to the rapid switching. The loss in signal intensity is minimized by choosing a large filterwidth (1 MHz) together with a large spectral width (100 kHz).¹⁴



Figure 11 500 Mhz proton spectra of a 2 mM solution of sucrose in 90% H2O/10% D2O, obtained after a single pulse excitation with regular (high Q) observation (a and c) and with Q-switching during acquisition (b and d). In each case 8 scans were acquired with a data sampling interval t_s of 20 µs and in the Q-switching experiments the interval t_{low} was 17 µs (off ratio 0.85).

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4.5 Selective excitation and Q-Switching



Figure 12 Pulse scheme for selective excitation with a Gaussian pulse and Q-Switching.

Radiation damping can also interfere with frequency selective excitation pulses. If the amplitude of the field generated by the coupling of a strong NMR signal with the receiver coil is of the same order as the amplitude of the RF field, radiation damping will degenerate the performance of the selective excitation pulse³.

Recently, Otting et al.¹⁵ have successfully employed Q-Switching to overcome the effects of radiation damping in selective excitation of the water resonance. By breaking up a shaped pulse in a DANTE-like fashion (see Figure 12) free precession periods are generated in which the Q of the probe is switched low, while during the RF pulses the probe is in the high Q mode. In doing so, the individual pulse elements of the shaped pulse require an increased amplitude, as compared to its continuous version, which therefore more readily overcome the counteracting effect of radiation damping. Radiation damping is further suppressed by switching to a low Q value during the free precession intervals.

The ability to selectively excite water with Q-Switched selective pulses enables the selective observation of water-protein NOEs and ROEs in one-dimensional experiments, analogous to cross sections of the two-dimensional experiments, and two-dimensional NOE, ROE and TOCSY correlations which are identical to the two-dimensional cross sections of the corresponding 3D experiments¹⁵.

A Q-Switched selective pulse can be derived from any excitation profile by inserting elements with zero amplitude in the desired waveform. This can be implemented either via pulse length or pulse amplitude modulation. In the case of pulse length modulation the length of the individual pulse elements is modulated according to the desired profile by explicitly writing each pulse length in the pulse program. Q-Switching is then applied during the delays in-between the pulse elements.

Amplitude modulation is achieved by using the shaped pulse feature. However, once the shaped pulse is invoked by the pulse programmer (e.g. via :sp1), it is not possible to switch the quality factor between high and low while this shaped pulse is being executed. In order to make the loop,

containing the Q-Switching statements, and the shaped pulse run in parallel, the shaped pulse is instead executed as a composite pulse decoupling (cpd) program. For details on the pulse programming of Q-Switched selective pulses please refer to the appendix of this manual.

5 References

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6 Appendix

6.1 Definitions for Q-Switching

Add the following definitions to the preamble of the pulse programs for experiments with Q-Switching or add these definitions to the *Avance.incl* file.

#define HIGHQ setnmr8^7	;switch probe to high Q mode (default)
#define LOWQ setnmr8 7	;switch probe to low Q mode

6.2 Inversion Recovery T₁ measurements

;t1irqp ;T1 measurement using inversion recovery ;with Q-Switching during recovery delay ;ref. C.G. Anklin et al., J.Mag.Reson., B106, 199, 1995

#include <Avance.incl>
#define HIGHQ setnmr8^7
#define LOWQ setnmr8|7

;switch probe to high Q mode (default) ;switch probe to low Q mode

```
1
       ze
2
       d1
       p2 ph1
       3u LOWQ
       vd
       3u HIGHQ
       p1 ph2
go=2 ph31
d11 wr #0 if #0 ivd
lo to 1 times 14
exit
ph1=02
ph2=0 0 2 2 1 1 3 3
ph31=0 0 2 2 1 1 3 3
;pl1 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;p2 : f1 channel - 180 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
;d11: delay for disk I/O
                                         [30 msec]
;vd : variable delay, taken from vd-list
```

;L4: 14 = number of experiments = number of delays in vd-list ;NS: 8 * n ;DS: 4 ;td1: number of experiments

;define VDLIST ;this pulse program produces a ser-file (PARMOD = 2D)

6.3 Noesy with Q-Switching during evolution

;noesysh11qp
;2D homonuclear correlation via dipolar coupling
;dipolar coupling may be due to noe or chemical exchange.
;phase sensitive using States et al. method
;water suppression using 1-1 pulse sequence
;with Q-Switching during t1
;ref. C.G. Anklin et al., J.Mag.Reson., B106, 199, 1995

#include <Avance.incl>
#define HIGHQ setnmr8^7
#define LOWQ setnmr8|7

;switch probe to high Q mode (default) ;switch probe to low Q mode

```
10=td1*0.5
```

1 ze 2 d1 d11 3 d11 4 p1 ph1 3u LOWQ d0 3u HIGHQ p1 ph2 d8 p1 ph3 d19 p0 ph4:r go=2 ph31d1 wr #0 if #0 ip1 zd lo to 3 times 2 d11 id0 ip31 d11 ip31 lo to 4 times 10 exit

ph1=0.2ph2=000000000 22222222 ph3=0 0 2 2 1 1 3 3 ph4=2 2 0 0 3 3 1 1 ph29=0 ph31=0 2 2 0 1 3 3 1 20023113 ;pl1 : f1 channel - power level for pulse (default) ;p0 : f1 channel - 90 degree high power pulse use for fine adjustment ;p1 : f1 channel - 90 degree high power pulse :d0 : incremented delay (2D) [3 usec] ;d1 : relaxation delay; 1-5 * T1 ;d8 : mixing time ;d11: delay for disk I/O [30 msec] :d19: delay for binomial water suppression d19 = (1/(2*d)), d = distance of next null (in Hz);L3: loop for phase sensitive 2D using States et al. method: 13 = td1/2;in0: 1/(1 * SW) = 2 * DW:nd0: 1 :NS: 8 * n :DS: 16 ;td1: number of experiments ;MC2: States

6.4 Q-Switched Selective Pulse

In the case of Q-Switched selective pulses a selective pulse is applied in a DANTE type fashion and the quality factor of the probe is switched to low in between the separate pulse elements in order to suppress radiation damping.

Any desired pulse profile can be executed as a Q-Switched selective pulse by inserting elements of zero amplitude in the shaped profile. This can be implemented either via pulse length or amplitude modulation. In the case of pulse length modulation the length of each pulse element is explicitly written in the pulse program and Q-Switching is applied during the delays in between the pulse elements. Amplitude modulation is achieved using the shaped pulse feature and one possible way to implement Q-Switched selective pulses using shaped pulses is shown below.

Pulse elements with zero amplitude are inserted into the shaped pulse by using Bruker's *SHAPE* program by following the steps below:

- 1. generate the desired waveform,
- 2. write the profile to an ASCII file,
- 3. insert the zero amplitude lines in this ASCII file,

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- 4. read the file back into the *em SHAPE* program and
- 5. write it out as a shaped pulse.

A shaped pulse consists of a series of N elements, and the duration τ of each element is determined by the total time allotted to the pulse (e.g. p31:sp1) divided by the number of elements ($\tau = p31/N$). A desired delay δ between the individual pulses is inserted in the shaped pulse by adding δ/τ lines of zero amplitude in the sequence. An simple example is shown below for an eight-element Gaussian pulse in which three zero amplitude elements are inserted after each line, resulting in a profile consisting of 32 elements.

Shaped pulse file:

RFVERSION_F 15.16959095 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 40.73686218 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 76.38292694 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 100.000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 100.000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 76.38292694 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 40.73686218 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 15.16959095 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000 0.00000000 0.0000000

In order to switch the quality factor during the zero amplitude elements of the shaped pulse, a composite pulse decoupling sequence is used to execute this pulse, which enables the Q-Switching to run simultaneously with the shaped pulse. The switching of the quality factor is contained in a loop which is timed such that the periods in which the Q is low coincide with the zero amplitude elements of the pulse.

;qsel ;Q-Switched selective pulse ;ref. G. Otting et al., J.Mag.Reson., B107, 192, 1995 #include <Avance.incl> #define HIGHO setnmr8^7 ;switch probe to high Q mode (default) #define LOWQ setnmr8|7 ;switch probe to low Q mode 1 ze 2 d1 20u pl2:f1 ;pl2 sets amplitude for shaped pulse (2u ph1):f1 ;set phase for cpd 2u cpds1:f1 ;start cpdprg1=qsel 3 :d31=p31/N d31 3u LOWQ ;switch to low Q d30 ;d30=n*d31 - 6u 3u HIGHQ ;switch to high Q loop to 3 times 11 :loop 11 times 4u do:f1 go=2 ph31wr #0 exit ph1=0ph31=0 ;d31=p31/N, N=number of elements in shaped pulse ;d30=n*d31 - 6u, n=number of zero elements inserted after each pulse :p31=length of shaped pulse ;11=number of non-zero pulse elements ;cpdprg1=qsel ;spname1=name of shaped pulse ; adjust pl2 to obtain 90 degree pulse for a given pulse length p31

The cpd program allows the shaped pulse to be executed in parallel to the Q-Switching.

cpd program qsel

#addphase

1 p31:sp1:0 jump to 1