Typical Pulses for the 5 mm CryoProbe™ 500MHz and 600MHz

History:

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1. Purpose

Safe operation of a NMR probe requires that the power and the durations of RF pulses do not exceed specified values. This document provides values for safe operation of the 5mm TXI CryoProbe™ at 500MHz and 600MHz.

2. Scope

All 5mm TXI CryoProbe™ at 500MHz and 600MHz.

3. Reference to Documents

None.

4. Implementation

4.1 Introduction

The following table shows values for pulses, which provide safe operation[1)] with a Bruker 5mm CryoProbe™.

The given values are related to the power handling of a 5mm CryoProbe™. The effect of possible heating of the sample is not taken into account.

Please note that the given values provide safe operation only, when

- standard pulse programs from the Bruker pulse program library are used, and
- the repetition rate, which is about ***d1+aq*** has a minimum period of 1s.

Certain segments in a pulse sequence, like a spin lock or a decoupling sequence, are applied at a given RF power level. The maximum allowed power for those segments is expressed by the corresponding pulse length. Example:

> *^{1}H TOCSY spin lock: 200 msec @ 25 msec. This means that the maximum length of the spin lock sequence is 200 msec, and the allowed ^{1}H power level corresponds to a 90 deg. pulse width of 25 msec. A power level corresponding to a 90 deg. pulse which is shorter than 25 msec is not allowed.*

4.2 Pulse and power recommendations

Note: All values require a minimum repetition period *d1+aq* of 1sec [2)]
Important: observe the separate notes on the following pages!

	5mm 500MHz TXI CryoProbe™	5mm 600MHz TXI CryoProbe™
^{1}H		
hard pulse [3)] (max. length 360°)	8.0 µsec	8.0 µsec
hard pulse for lossy samples	Power level corresponding to 8.0 µsec pulse for non-lossy sample	Power level corresponding to 8.0 µsec pulse for non-lossy sample
trim pulse p28 [4)]	2 msec @ 10 µsec	2 msec @ 10 µsec
TOCSY spin lock [5)]	200 msec @ 25 µsec 400 msec @ 35 µsec	200 msec @ 25 µsec 400 msec @ 35 µsec
ROESY spin lock	Up to CW for power level corresponding to a 100 µsec pulse	Up to CW for power level corresponding to a 100 µsec pulse
WALTZ16 decoupling during 13C-detection	Up to CW for power level corresponding to a 100 µsec pulse	Up to CW for power level corresponding to a 100 µsec pulse
DIPSI2-decoupling in triple resonance	400 msec @ 50 µsec	400 msec @ 50 µsec
^{13}C		
hard pulse [6)] (max. length 360°)	15.0 µsec	15.0 µsec
trim pulse [5)]	2 msec @ 25 µsec	2 msec @ 25 µsec
CC spin lock [5)]	20 msec @ 25 µsec	20 msec @ 25 µsec
GARP decoupling [7)]	140 msec @ 65 µsec	140 msec @ 55 µsec
selective pulses [8)]	Q5: 320 µsec Q3: 256 µsec CHIRP: 2 ms @ 25 µsec	Q5: 320 µsec Q3: 256 µsec CHIRP: 2 ms @ 25 µsec
^{15}N		
hard pulse [6)] (max. length 360°)	40.0 µsec	40.0 µsec
WALTZ16 decoupling [7)]	140 msec @ 200 µsec	140 msec @ 170 µsec
CPMG T2 [9)]	250 msec @ 80 µsec (see warning [9)])	250 msec @ 80 µsec (see warning [9)])
^{2}H		
hard pulse (max. length 360°)	150 usec	150 usec
WALTZ16 decoupling	100 msec @ 250 µsec	100 msec @ 250 µsec
Z-Gradient		
Absolute max. current [10)]	10 A	10 A
Max.overall length [11)]	10 ms @ 10 A	10 ms @ 10 A

Table 1

4.3 Notes

[1)] Although the values given do not necessarily define the actual limits, these conditions have been determined to provide safe operation and are valid unless superseded in whole or in part by (1) a more recent version of this document, (2) a factory document pertaining to the specific probe, or (3) written approval by BRUKER BioSpin AG. Operation in excess of the conditions given is not permitted and will void the warranty as it may result in a damage to the CryoProbe.

[2)] Repetition period related isssues:
a) In any case, the power level for a given pulse length (which must be equal or shorter than the specified pulse length value) must never exceed the power maximum given in Table 1.
b) The pulse length values given in Table 1 are based on a repetition period of approximately 1sec. This defines and limits the average power to which the probe may be exposed. Operation with longer repetition periods is allowed without additional restrictions, provided the pulse lengths are still limited according to the values given in Table 1.

[3)] Non-lossy samples are assumed, such as organic solvents or water without salt.

[4)] A number of inverse correlation experiments use the proton trim pulse *p28*, like the pulse program *invietgpsi (XWINNMR up to version 3.1) or hsqcetgpsi (XWINNMR version 3.5)*. According to our experience this trim pulse is only rarely required. Verify if any improvement is necessary or obtained using this pulse.

[5)] An experiment might contain a spin lock followed by a trim pulse. Note that the total length of spin lock and trim pulse must not exceed the value which is allowed for the spin lock only.

[6)] When hard pulses are applied simultaneously on the ^{13}C and ^{15}N channel, the power on both, the ^{13}C and the ^{15}N channel, has to be reduced by 3 dB each.

[7)] Simultaneous decoupling of ^{13}C and ^{15}N requires that reduced power is used on both channels. 3 dB less power should be used for both ^{13}C and ^{15}N. For simultaneous decoupling it is recommended to use optimised conditions for adiabatic decoupling on ^{13}C.

[8)] Pulses Q5 and Q3 are used in triple resonance experiments. The 2 ms CHIRP pulse is used in HSQC experiments for refocusing. For shaped selective pulses there are usually no restrictions, as long as the peak power of the shape does not exceed the power limit of a hard pulse. When using non-standard pulses, in addition to the peak power, it should be also verified that the averaged power over the pulse length does not exceed any of the power limits (compare to the listed limits for pulses with a comparable duration).

[9)] The pulse sequence *invit2etf3gpsi (XWINNMR up to version 3.1) or hsqct2etf3gpsi (XWINNMR version 3.5)*. The length of the CPMG element is *d20* and should not exceed 250

msec. The 180 deg. pulse is *p30* at a power level *pl23*, the pulse *p30* should not be shorter than 160 µsec (180 deg. pulse, applied at a power level corresponding to a 90 deg. pulse of 80 µsec). The given value is true only, when the pulse p30 is part of a CPMG sequence with an inter-pulse delay of 900 µsec (expressed by *d21*2* in the pulse sequence *invit2etf3gpsi*). Warning: Never apply the above power level and full uninterrupted duration in a spin lock sequence.

10) The absolute max. gradient current $\boldsymbol{I_{max}}$ is listed in Table 1.

11) It is permissible to apply $\boldsymbol{I_{max}}$ for the listed maximum overall length $\boldsymbol{T_{max}}$. The overall length of the gradients is the sum of all gradients applied during a repetition period.

A gradient sequence which has, within a repetition period, an overall length $\boldsymbol{T_G}$ which is longer than $\boldsymbol{T_{max}}$, is still permissible if the maximum gradient current is reduced to $\boldsymbol{I_G}$, according to the following equation:

$$I_G = I_{\max} * \sqrt{T_{\max} / T_G}$$

In a more general formulation (using the values of $\boldsymbol{I_{max}}$ = 10 A and $\boldsymbol{T_{max}}$ = 10 msec for clarity), for N pulses within any repetition (one second) period, the following condition must hold ($\boldsymbol{I_{Gi}}$, $\boldsymbol{T_{Gi}}$ denote the current and duration of the i-th gradient pulse):

$$\sum_{i=1}^{N} T_{Gi} {I_{Gi}}^2 \le T_{\max} * \left(I_{\max}\right)^2 = 10ms \cdot \left(10A\right)^2 = 1000 \cdot msA^2$$

Examples:

1. For an overall gradient length of $\boldsymbol{T_G}$ = 20 ms within any one second period, the maximum gradient current $\boldsymbol{I_G}$ is 7.07 A.
2. A pair of gradient pulses, consisting of a first pulse with a current of 10 A and a length of 5 msec, and a second pulse with a current of 5 A and a length of 20 msec is just permissible.
3. A DC current of 1 A is just permissible.