

Typical Pulses for the Inverse 5 mm CryoProbe™

500 MHz and 600 MHz

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History:

Index	Date	Changes	Initials
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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 5 mm TXI/TCI CryoProbe™ at 500 MHz and 600 MHz.

2. Scope

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

3. Reference to Documents

None.

4. Implementation

4.1 Introduction

The following table shows values for pulses, which provide safe operation¹⁾ with a Bruker 5 mm CryoProbe™.

The given values are related to the power handling of a 5 mm 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 1 s.

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:

¹H TOCSY spin lock: 200 ms @ 25 s. This means that the maximum length of the spin lock sequence is 200 ms, and the allowed ¹H power level corresponds to a 90° pulse width of 25 s. A power level corresponding to a 90° pulse which is shorter than 25 s is not allowed.

4.2 Pulse and power recommendations

Note: all values require a minimum repetition period $d1 + aq$ of 1s²⁾.

Important: observe the separate notes on the following pages!

	5 mm 500 MHz TXI/TCI CryoProbe™	5 mm 600 MHz TXI/TCI CryoProbe™
¹ H		
hard pulse ³⁾ (max. length 360°)	8.0 s	8.0 s
hard pulse for lossy samples	Power level corresponding to 8.0 s pulse for non-lossy sample	Power level corresponding to 8.0 s pulse for non-lossy sample
trim pulse <i>p28</i> ⁴⁾	2 ms @ 10 s	2 ms @ 10 s
TOCSY spin lock ⁵⁾	200 ms @ 25 s 400 ms @ 35 s	200 ms @ 25 s 400 ms @ 35 s
ROESY spin lock	Up to CW for power level corresponding to a 100 s pulse	Up to CW for power level corresponding to a 100 s pulse
WALTZ65 decoupling during ¹³ C-detection	Up to CW for power level corresponding to a 100 s pulse	Up to CW for power level corresponding to a 100 s pulse
DIPSII-decoupling in triple resonance	400 ms @ 35 s	400 ms @ 35 s
¹³ C		
hard pulse ⁶⁾ (max. length 360°)	12.0 s	12.0 s
trim pulse ⁵⁾	2 ms @ 25 s	2 ms @ 25 s
CC spin lock ⁵⁾	20 ms @ 25 s	20 ms @ 25 s
GARP4 decoupling ⁷⁾	140 ms @ 65 s	140 ms @ 55 s
selective pulses ⁸⁾	Q5: 384 s Q3: 307 s CHIRP: 2 ms @ 25 s	Q5: 320 s Q3: 256 s CHIRP: 2 ms @ 25 s
¹⁵ N		
hard pulse ⁶⁾ (max. length 360)	35.0 s	35.0 s
GARP4 decoupling ⁷⁾	140 ms @ 200 s	140 ms @ 170 s
CPMG T2 ⁹⁾	250 ms @ 63 s (see warning ⁹⁾)	250 ms @ 52 s (see warning ⁹⁾)
² H		
hard pulse (max. length 360°)	68 s	68 s
WALTZ64 decoupling	100 ms @ 250 s	100 ms @ 250 s
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 damage to the CryoProbe.
- 2) Repetition period related issues:
 - 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 1 s. 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 or Topspin). 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 optimized 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) ^{15}N T_2 pulse sequence *invit2eff3gpsi* (XWINNMR up to version 3.1) or *hsqct2eff3gpsi* (XWINNMR version 3.5 and Topspin): The length of the CPMG element is *d20* and should not exceed 250 ms. The 180° pulse is *p30* at a power level *pl23*, the pulse *p30* should not be shorter than 104 μs @ 600 MHz and 126 μs @ 500 MHz (180° pulse, applied at a power level corresponding to a 90° pulse of 52 μs and 63 μs , respectively). Increase the recycle delay to > 2.5 s. The given value is true only, when the pulse *p30* is part of a CPMG sequence with an inter-pulse delay of 900 μs (expressed by *d21·2* in the pulse sequence *hsqct2eff3gpsi*).

Warning: Never apply the above power level and full uninterrupted duration in a spin lock sequence.

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

11) It is permissible to apply I_{max} for the listed maximum overall length 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 T_G which is longer than T_{max} , is still permissible if the maximum gradient current is reduced to I_G , according to the following equation:

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

In a more general formulation (using the values of $I_{\text{max}} = 10 \text{ A}$ and $T_{\text{max}} = 10 \text{ ms}$ for clarity), for N pulses within any repetition (1 s) period, the following condition must hold (I_{Gi} , T_{Gi} denote the current and duration of the i -th gradient pulse):

$$\sum_{i=1}^N T_{Gi} I_{Gi}^2 \leq T_{\text{max}} \cdot (I_{\text{max}})^2 = 10 \text{ ms} \cdot (10 \text{ A})^2 = 1000 \cdot \text{msA}^2$$

Examples:

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