Supplementary Material: Broadband Excitation Pulses for High-Field Solid-State Nuclear Magnetic Resonance Spectroscopy

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1. Scripts

Included with this supplementary material are a series of files for generating and testing $^{\mathrm{OC}}$EX pulses using SIMPSON. Each script file is executed using the command:

    simpson script.in pulse_length

where `script.in` is the name of the input script and `pulse_length` is the desired length of the $^{\mathrm{OC}}$EX pulse. Inside each script file are several parameters that should be set before execution, including the magic-angle-spinning frequency, the magnetic field (specified as the ^{1}H frequency), and the number of pulses to be generated at each stage. The default values for other variables should be adequate for most situations. As later scripts use the output of previous scripts, all scripts should be executed from within the same directory. In addition, the RF inhomogeneity file needs to be in the same directory.

Each script creates a subdirectory for its output. The individual shape files that are generated are labeled as `EX-spinning frequency (Hz)-pulse length (in μs)-theoretical transfer efficiency.dat`. The theoretical transfer efficiency is used to distinguish different pulses. Although it is not guaranteed to be unique, it is precise enough (10 to 12 digits) that it functions reasonably well as a serial number.

1.1. General Scripts

`lorentz5p` : RF inhomogeneity file. Needed for later stages of optimization and testing.

`shape2bruker.all` : TCL script to convert SIMPSON shape files (with amplitudes in Hz) into Bruker format (with amplitudes in percent of some maximum value). Executed as "`tclsh shape2bruker.all pulse_length ?<maxrf>?`" where `maxrf` is an optional parameter that can be used to ensure that all pulses are scaled to the same RF amplitude value. This script generates a new directory (`Bruker-EX-pulse_length`) containing the output files.

1.2. $^{\mathrm{OC}}$EX Design

`EX-OC1.in` : Initial script for generating $^{\mathrm{OC}}$EX pulses. A narrow band optimization for excitation.

`EX-OC2.in` : Uses output from previous script. Adds chemical shift offsets to ensure excitation over the desired chemical shift range.

`EX-OC3.in` : Uses output from previous script. Adds an RF inhomogeneity profile.

`EX-OC4.in` : Uses output from previous script. Sets amplitudes to a constant value (50 kHz) and recalculates.

`EX-test.in` : Uses output from previous script. Used to test pulse performance.

2. Pulses

$^{\mathrm{OC}}$EX pulses are designed to convert I_z magnetization to I_x magnetization, and $^{\mathrm{OC}}$FB pulses convert I_x magnetization to I_z magnetization. Consequently, when used in a pulse sequence the pulse phase needs to be adjusted by 90° relative to conventional hard excitation/flip-back pulses.

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2.1. ^{OC}EX

The $^{\mathrm{OC}}$EX shape files are labeled as `EX-spinning frequency (Hz)-pulse length (in μs)-theoretical transfer efficiency`. The shape files are provided in SIMPSON format (indicated by the `.dat` suffix) and Bruker format (indicated by the `.bru` suffix).

The Bruker shapes have the same maximum RF amplitude (50 kHz). To setup the pulses, first calibrate a 50 kHz RF field for the relevant channel (i.e., a 5 μs 90° pulse). Ideally, the $^{\mathrm{OC}}$EX pulses should work with this power level, but in practice you may want to optimize the power level for best performance.

2.2. ^{OC}FB

The $^{\mathrm{OC}}$FB shapes are simply time-reversed versions of the $^{\mathrm{OC}}$EX shapes with an additional 180° phase change. The change in phase is required so that the pulses convert I_x magnetization to I_z magnetization (instead of converting I_x magnetization to $-I_z$ magnetization). The $^{\mathrm{OC}}$FB shape files are labeled as `FB-spinning frequency (Hz)-pulse length (in μs)-theoretical transfer efficiency`. The shape files are provided in SIMPSON format (indicated by the `.dat` suffix) and Bruker format (indicated by the `.bru` suffix).

The Bruker shapes have the same maximum RF amplitude (50 kHz). To setup the pulses, first calibrate a 50 kHz RF field for the relevant channel (i.e., a 5 μs 90° pulse). Ideally, the $^{\mathrm{OC}}$FB pulses should work with this power level, but in practice you may want to optimize the power level for best performance.