Magpie exercises

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22nd July 2022

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1 Introduction

In this document, some example exercises for teaching with Magpie are listed. They range from introductory examples for student's first steps in magnetic resonance, and also some studies of more advanced effects.

For each example, the suggested pulse sequence and sample file are listed. Then, a list of actions/steps is listed. It is suggested to embed this in a broader explanation of NMR effects, and how NMR experiments work.

Feel free to use these exercises, or an adaption of them, for your teaching needs. If you have suggestions for additions, do not hesitate to contact us.

2   Basic setup

Sample: `Ethanol.txt`.
   Pulse sequence: `onePulse.csv`

2.1   Introduction

In this exercise an initial introduction into basic spectrometer setup is given. This guides through all the steps to get a high-quality ^{1}H NMR spectum of an ethanol sample.
   The topic addressed are:

- Gain

- Spectrometer offset

- Spectral width

- Acquisition time

- 90° pulse determination

- T_1 effects

2.2   Steps

Below is a list of suggested steps to follow.

- Record spectrum with default settings. (Optionally adopt the default settings to be less good.)

- Examine FID and spectrum.

- Optimize gain (single scan maximum at about 0.8 in FID)

- Optimize acquisition time.

- Optimize offset, to have spectrum centred.

- Reduce spectral width to have a nice fitting spectrum. Keep to total acquisition time constant.

- Optimize pulse length. Acquire a series of spectra with different pulse lengths (as an array) and determine the signal maximum. A pitfall here could be that the gain was pre-optimize before finding the 90° pulse.

3   T1 determination

Sample: `Ethanol.txt`.

   Pulse sequence: `invRecovery.csv` and `satRecovery.csv`.

3.1   Introduction

Using the optimized settings of section 2, the T_1 is determined for the sample. Firstly, it is done using inversion recovery, followed by the repeat of this using saturation recovery. The students should learn the requirement for inversion recovery to wait 3-5 times T_1 between scans, before the T_1 is established! Then we move to saturation recovery, to show if can be used in a more effective manner. Note that Magpie uses a perfect saturation block, and not a series of pulses. The disadvantage of saturation recovery, especially if the sample T_2 approaches the T_1 are not taken into account.

   The topic addressed are:

- T_1 determination using inversion recovery.

- (Addition: use composite pulse for inversion.)

- T_1 determination using saturation recovery.

3.2   Steps

Below is a list of suggested steps to follow.

- Load the `invRecovery.csv` sequence.

- Using the optimized setting for ethanol, test the inversion recovery by setting the delay at a low value. This should give an inverted spectrum.

- Ste the delay at a large value to show the signal positive again.

- Manual try and find the zero crossing.

- Set up an array of experiments from short to long recovery times. Analyse this data in ssNake to determine the T_1.

- Repeat the experiment with a very short recycle delay. How does this impact the recovery curve? How reliable would this analysis be?

- With the optimal setting, move to the `satRecovery.csv` sequence.

- Repeat the experiment with the array of the recovery times. Analyse the data in ssNake.

- Repeat the experiment with a very short recycle delay. Observe the difference between this fit result and that for the inversion recovery sequence with too short recycle delay.