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A useful workflow

to estimate T_1 for quantitative NMR analysis

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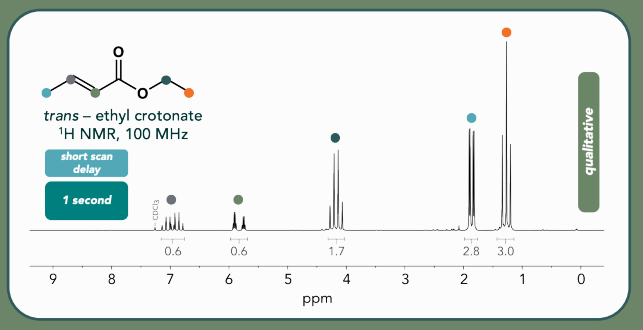
The spin-lattice or longitudinal relaxation time constant, T_1, characterizes the rate at which the spin magnetization (M_z) returns to thermal equilibrium. The T_1 is a determining factor in the optimization of the scan delay, which has significant importance in applications involving quantitative NMR (qNMR). The goal of this workflow is to ensure the optimization of the scan delay for acquisition of qNMR data. In our instrument, the first step is to run a 1D spectrum, adjust the phase of signals, and integrate the signals of interest.

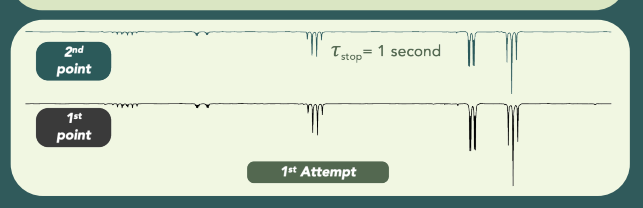


2

The second step is to set up the quick T_1 experiment (select the T_1 experiment on the main menu), adjust both the number of steps and number of scans to 2. Note that if the sample is dilute then the scans may have to be increased, since insufficient SNR will yield inaccurate results.

Since the T_1 is unknown, we recommend to set the scan delay to 60 seconds and tau stop to 1 second. Manipulate the tau stop to find the null point or the point at which the phase of the signals of interest invert. After the experiment, view the two spectra to observe if a change in phase of the desired signals has occurred. Note that if the signal is still negative (like in spectrum on the right) you will need to increase the tau stop, and if it is still positive you will need to reduce the tau stop.

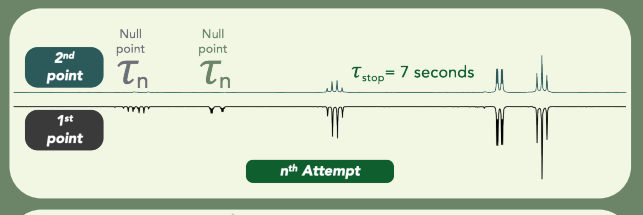
Parameters of quick T_1 experiment	Number of steps	Number of scans	Scan delay	Tau stop (τ_{stop})
	2	2	60 s	1 s



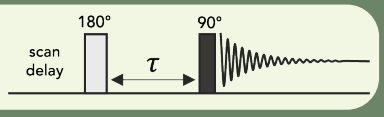
3

After finding the longest null point of the signals of interest (7 seconds in the spectrum on the right), the third step is to insert that value for τ_n (7 seconds) into the formula below to estimate the T_1 value.

Formula	Estimated Null point		Estimated		Scan delay
	τ_n	÷ln(2) →	T_1	×5 – 7 →	
	7 seconds		~10 seconds		~60 seconds

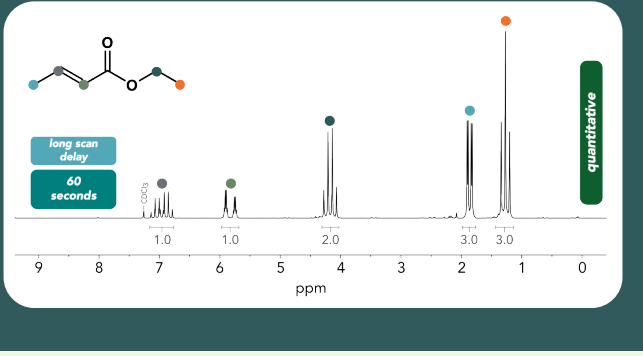


Inversion Recovery Pulse Sequence for T_1 measurements



4

From the longest estimated T_1 value in the sample (determined to be 10 seconds) adjust the scan delay accordingly (optimized to 6 xT_1 = 60 seconds for this sample). The last step is to re-run the 1D spectrum with the optimized scan delay. With this workflow, initial qualitative data can be updated to quantitative data through accurate integrals as seen in the spectrum on the right.



Read more about T_1's here:
www.nanalysis.com/nmready-blog/2022/6/29/part-1-t1-relaxation-definition-measurement-and-practical-implications
www.nanalysis.com/nmready-blog/2020/9/28/oxygen-how-does-it-affect-your-t1-times