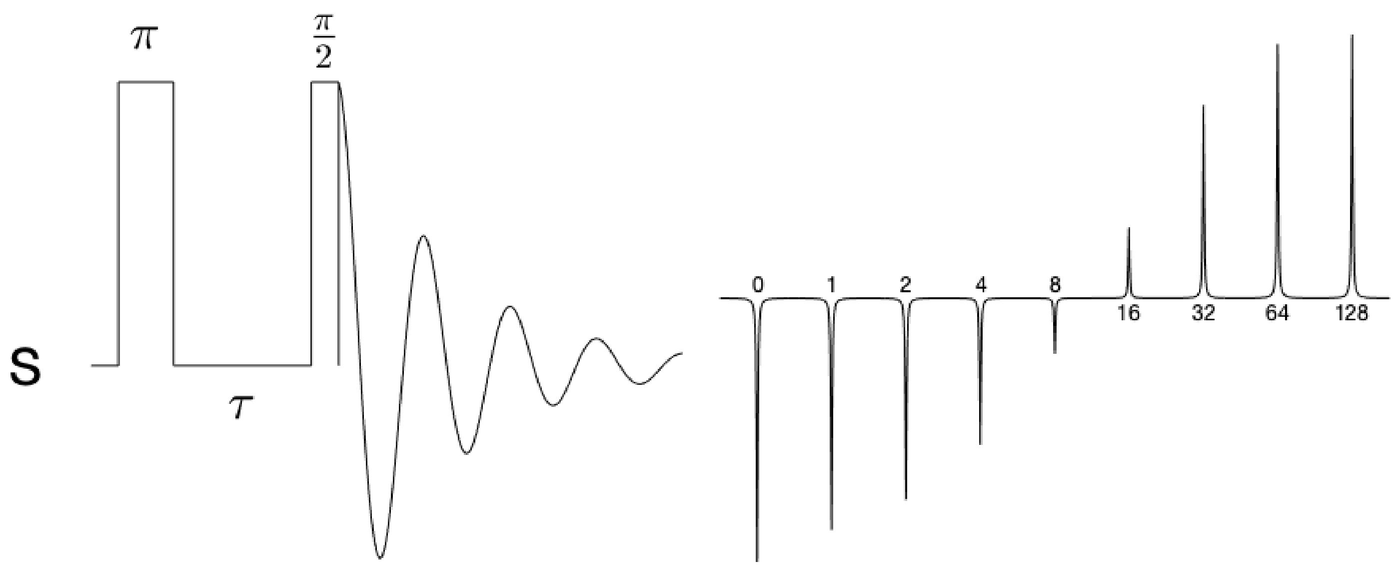
June 2022 NMR Topic of the Month: T_1 Relaxation

What is T_1 relaxation?

This is the spin-lattice or longitudinal relaxation, and is a measure of the time required for the system to reach thermal equilibrium. The T_1 of a system provides information about the targets' motion and dynamics. This information is often valuable on its own, but is also used to provide contrast in MRI.



How does one measure the T_1 time?

You do an inversion-recovery experiment (like the one shown above on the left) where the tau delay is changed incrementally. The resulting array of spectra (shown above on the right where the numbers indicate the value of the tau delay in seconds) is then fit using non-linear regression to the model $y = A\left(1 - Bexp\left[-x/T_1\right]\right)$, where A is the absolute amplitude of the spectrum when the tau delay is zero and B should be 2. The value for B is left as a fitted parameter because it is impractical to acquire a true tau delay of 0 seconds, and allowing it to vary accounts for this (following fitting B will be less than 2).

What are some of the pitfalls for doing an inversion-recovery experiment?

There are several important things to keep in mind. First, the pulses should be well-calibrated for the conditions and sample; otherwise, erroneous non-exponential behavior can result. This includes correcting for peaks offset from the transmitter. Second, using compound or shaped pulses generally does not work well, instead rerun the experiment with a different offset. Third, if there is decoupling during the tau delay to ameliorate spin diffusion, be careful with your power level. Fourth, this experiment can take a while, so plan well. In the example above just the final tau delay is over two minutes long, the relaxation delay will be that long as well, and the acquisition will take time - it could be nearly 5 minutes per transient at that point. Fifth, the tau delay should be arrayed so that there are several negative and positive spectra, and should run past 99.9% recovery. In the above example, $T_1 \approx 15.9$ seconds, so $7T_1 \approx 111.4$ seconds < 128 seconds, and the zero crossing is at 11.0 seconds = $\ln(2)T_1$.

References

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