

## Measurement of Spin-Lattice Relaxation Time ( $T_1$ )

The most often used pulse sequence to measure spin-lattice relaxation time is the  $180^\circ - \tau - 90^\circ$  sequence (Figure 1.)

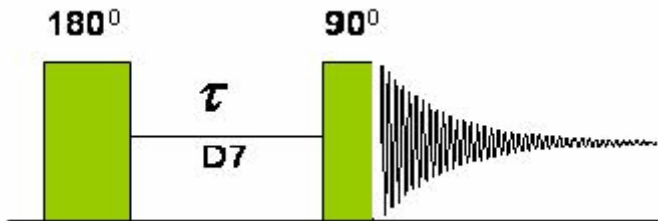


Figure 1. The pulse sequence to measure spin-lattice relaxation time. The  $D7$  delay corresponds to time  $\tau$ .

It is known also as the inversion recovery  $T_1$  measurements. At the time  $\tau = 0$  the  $180^\circ$  pulse inverts the magnetization vector  $M_z$ . After this the magnetization  $M_z$  lies along the negative  $z$  axis and  $M_z = -M_z$  Fig.2.

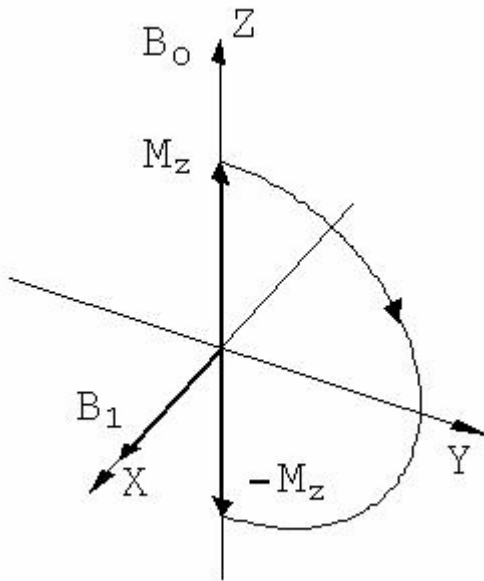


Figure 2. The inverted magnetization  $M_z$  after  $180^\circ$  pulse.

The spin-lattice relaxation makes the magnetization  $M_z$  increase (Figure 3) during  $\tau$  interval from  $-M_0$  throughout zero until it is back to original value  $M_z = M_0$ .

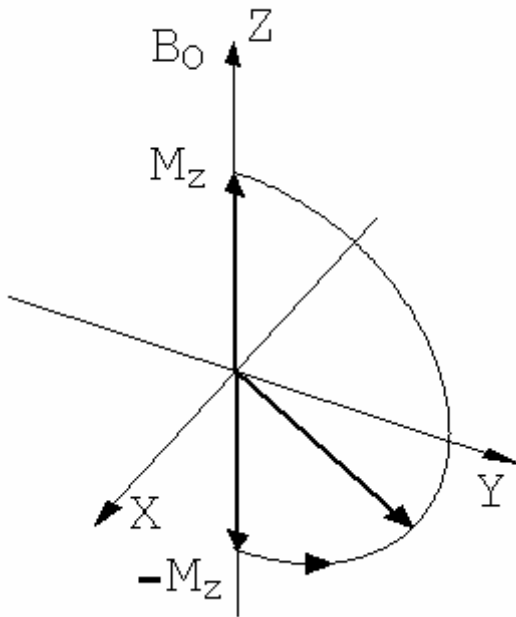


Figure 3. Magnetization  $M_z$  relaxes back to the original position after  $180^\circ$  pulse.

One can find the value of  $M_z$  at any time of  $\tau$  using the following formula:

$$M_z = M_0 \left( 1 - 2e^{-\frac{\tau}{T_1}} \right) \quad (1)$$

If at some time  $\tau$  following the  $180^\circ$  pulse, the  $90^\circ$  pulse is applied  $M_z$  is rotated around the X axis and will then lie somewhere along the Y axis. If the time  $\tau$  separating two following passages is short compared with  $T_1$  the two NMR signals have the same sign, and opposite sign when  $\tau > T_1$  Fig.4.

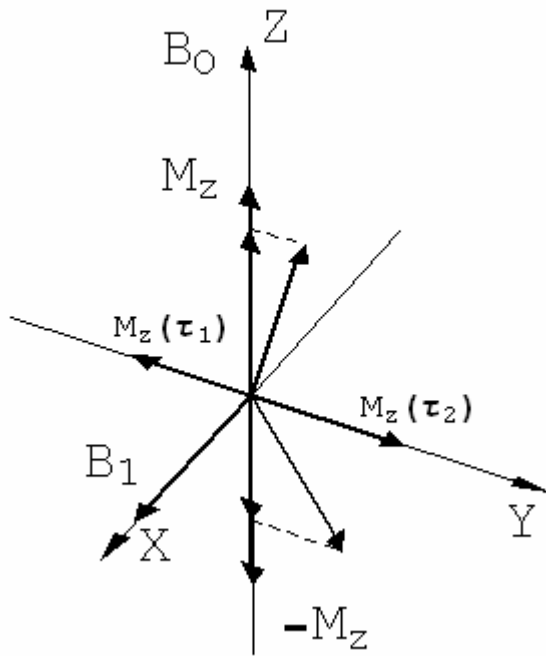


Figure 4. The magnetization  $M_z$  is transferred to Y axis by  $90^\circ$  pulse, negative  $M_z(\tau_1)$  and positive  $M_z(\tau_2)$

Finding  $T_1$  involves measurements of the signal amplitude for several different  $\tau$  intervals. Such magnitudes of amplitudes are depicted on Figure 5.

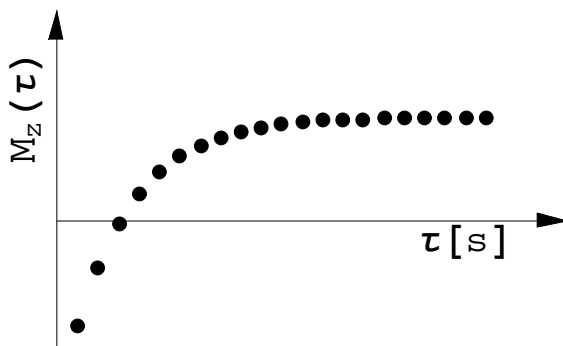


Figure 5. Spin-lattice magnetization recovery according to measurements.

Performing the curve fitting according to formula (1) will give  $T_1$ . It is known that formula (1) does not always describe correctly the magnetization recovery (this depends on molecular structure and dynamics), so the person performing the experiment needs to decide if the modified formula should be applied instead.

To protect quantitation and correct timing for most of the two-dimensional experiments on a daily basis, there is no need to run the time consuming full size  $T_1$  measurements. Instead the so called “null” method proves useful. In this method the time  $\tau = \tau_{null}$  for which  $M_z = 0$ , and signal disappeared needs to be found. The  $T_1$  can be estimated using the following formula:

$$T_1 = \frac{\tau_{null}}{\ln 2} \quad (2)$$

Again, it needs to be stressed that this a rough estimate. To run this experiment one needs to calibrate the  $90^0$  pulse (since the inversion recovery method is sensitive to pulse accuracy) and call the experiment: e.g. “rpar H1T1null.BBI”. The D7 delay in the Bruker software has a meaning of  $\tau$ . After  $\tau_{null}$  is found  $T_1$  is calculated.

[Experiment setup](#)

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