# F61: Nuclear magnetic resonance spectroscopy

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**Abstract**

*The goal of this experiment is to do research on the characteristics of the muon. In detail we want to determine the lifetime and polarization of cosmic muons, which would also prove parity-violation in the weak interaction. For all our measurements we have six layers of scintillators with metal in between. Furthermore we can add a homogeneous magnetic field so that the muon will do a larmor-precession around the direction of the field. This makes it possible to determine the larmor-frequency, the magnetic moment of the muon and the polarization. The evaluation was done with ROOT.*

## I. AUSWERTUNG

### 1. Measurement of relaxation times

Both the spin-spin and the spin-lattice relaxation time have been measured with the use of two different concentrations of Gadolinium solved in water, one solution with 500 water molecules per Gadolinium atom (Gd500) and the other containting 600 water molecules per Gadolinium atom (Gd600). The measured values were aquired by a fit of their respective fit functions $M_\perp(t) = M_\perp^0 \, e^{-\frac{t}{T_2}}$ for $T_2$ and $M_\parallel(t) = M_\parallel^0 \left(1 - 2\,e^{-\frac{t}{T_1}}\right)$ for $T_1$ applied to the measured data 1

|  | Gd500 | Gd600 |
|---|---|---|
| $T_2$ | $(99.8 \pm 0.5_{stat})\,\mathrm{ms}$ | $(129 \pm 1_{stat})\,\mathrm{ms}$ |
| $T_2(\mathrm{CP})$ | $(124.0 \pm 0.4_{stat})\,\mathrm{ms}$ | $(150.6 \pm 0.6_{stat})\,\mathrm{ms}$ |
| $T_1$ | $(118.8 \pm 2.2_{stat})\,\mathrm{ms}$ | $(135.8 \pm 1.2_{stat})\,\mathrm{ms}$ |

**Table 1:** *Measured Values*

We aquired a data point at 900ms echo time for the $T_1$ Gd500 measurement which we decided to exclude from the fitted dataset as it was way higher than one would theoretically expect. We found the reason for this to be the sensitivity of the measurement configuration to the background noise, because we changed the integrated over peak window before the aquirement of said data point. One theoretically expects $T_2(\mathrm{CP})$ to be larger than $T_1$ for both solutions, because the spin-spin interaction dominates $T_2$: Dipoles want to align in the energetically most favourable way, antiparallel. This alignment proceeds faster in comparison to the spin-lattice interaction

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important for the $T_1$ measurement. $T_1$ describes the average time needed for the mean magnetization to go over from antiparallel to parallel alignment with respect to the external magnetic field, this is microscopially described by single spins orienting themselves from $-1/2$ to $+1/2$. We furthermore observe the relaxation times of Gd500 to be shorter than for Gd600. Gadolinium is strongly paramagnetic and is magnetized at room temperature (Curie point at $\approx 19\,°C$). The form of paramagnetism exhibited by Gadolinium compounds derives from electrons, not protons, and is known as Curie paramagnetism. Because of electrons having $s = 1/2$, but a much smaller size than the proton, their gyromagnetic ratio is $\approx 657$ times larger. If the electrons remain unpaired in shells or bonding orbitals, the unbalanced spin produce a strong magnetic moment capable of inducing magnetic relaxation in nearby nuclei. The seven unpaired electrons in the $4f \rightarrow s_e = 7/2$ subshell therefore account for the elements strong paramagnetism. The presence of such large fluctuating paramagnetic moments in a solution thus has strong effects on the nuclear spin relaxation of the solvent water nuclei. Therefore, the more Gadolinium atoms available the more dipole-dipole interactions between the water molecules and the Gadolinium atoms are possible and the shorter is the relaxation time. Instead we measured exactly the opposite to be true 1. We therefore repeated our measurement for $T_2$(CP) and for $T_1$ with the Gd600 probe and a more narrow peak window to further exclude background noise. $T_2$(Cp) didn't change much, but the new value for $T_1$ was $T_1 = (251.9 \pm 4.7_{stat})$ ms and therefore met our theoretical expectations. Thus, again the use of the same configuration with a slightly more narrow peak window leads to a huge difference in measured values. The whole setup is therefore very sensitive to the integrated over peak window, which hence should be checked quite thouroughly in order to guarantuee reproducibility of results in this section.
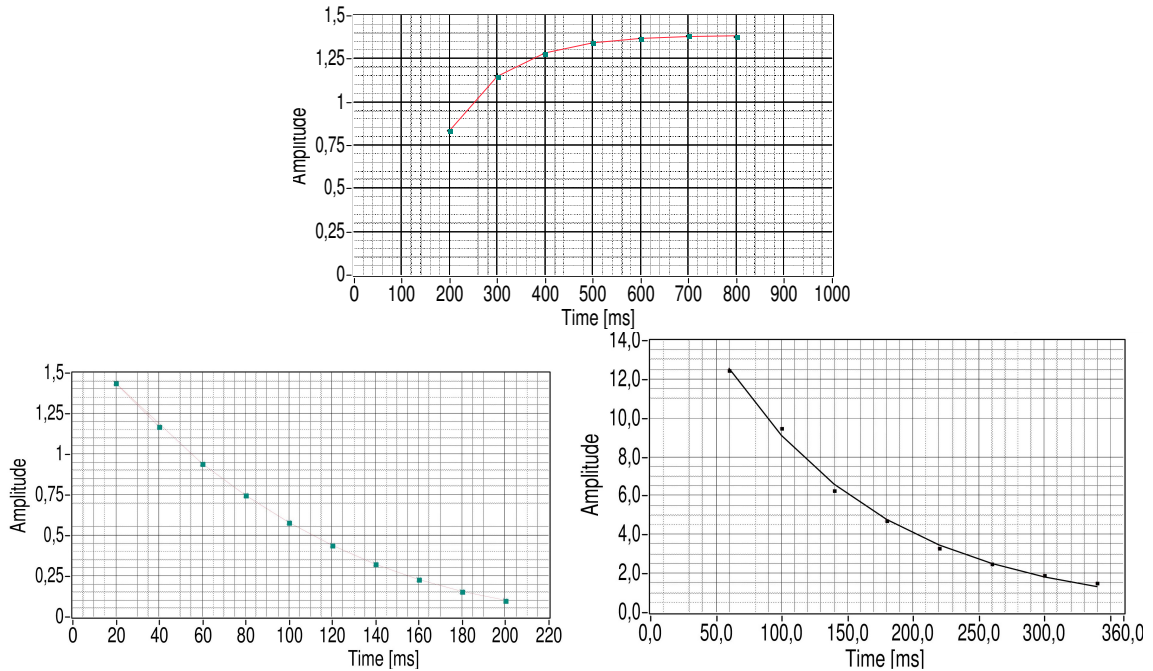


**Figure 1:** *In the top row: spin-lattice relaxation time $T_1$ in Gd500 with spin-echo method*
*From left to right in the bottom row: spin-spin relaxation time $T_2$ in Gd500 with spin-echo method and spin-spin relaxation time $T_2$ in Gd500 with the Carr-Purcell (CP) method*

## 2. Chemical shift

In order to identify the different simples A-E with the given chemical substances (Toluene, p-Xylene, Acetic acid, Fluoroacetone, Fluoroacetonitril) we applied a 90 °pulse on the respective samples and aquired via Fourier transformation a frequency spectrum as output signal in which the different larmor frequencies where observable. The sample was put into a rotating motion via compressed air in order to average out inhomogeneities withing the external magnetic field - the respective peaks got clearly more narrow and more distinct. Rotating the sample near the relaxation time though messes up the system such that we constantly calibrated the applied working frequency after every measurement to be at the order of $\nu_{work} = (506 \pm 20)$Hz. This was also neccessary because the experimental setup is not isolated very well such that drifts in the magneticfield due to temperature variation are, despite the short measurement time, not preventable. We furthermormeasured samples A+-E+ which additionaly contained the substance Tetramethylsilane (TMS). The hydrogen resonance line of TMS is located near the edge of the shown spectrum due its high chemical shift, we can thus use this line as a reference in order to distinguish between different samples. With the difference between the peaks of the respective samples and the reference peak we can identify every sample via 3: For sample A+ and D there
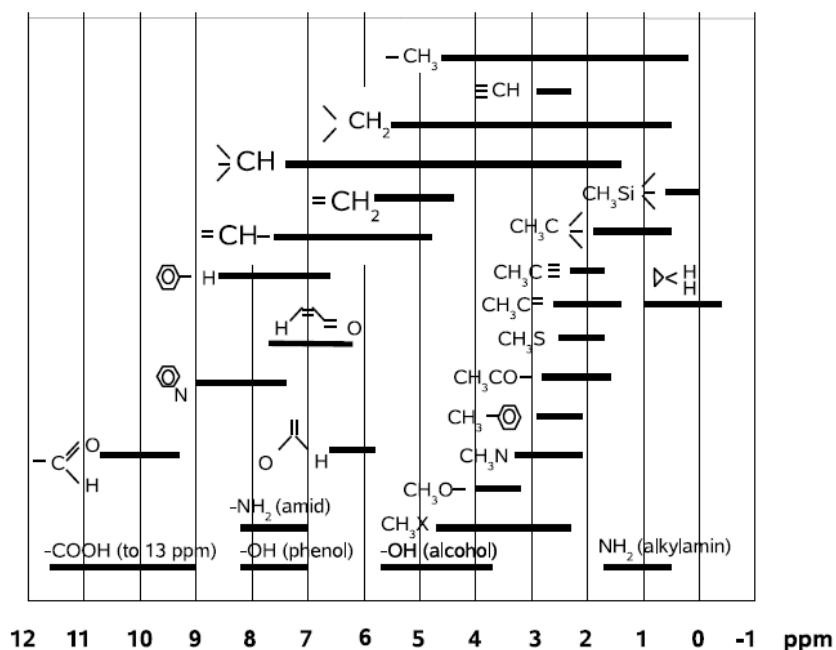


**Figure 2:** *Chemical shift of compounds relative to TMS [?].*

were no corresponding samples with/without TMS available such that we identified the TMS reference peak via the samples B+, C+, E+. We found the ppm position of said peak by averaging said samples to be at $TMS = (31.30 \pm 0.12)$ ppm. This value can in the following be used as a reference value for the sample D, where no D+ sample was available, and for identifying the reference value for A+, where no sample A was available.
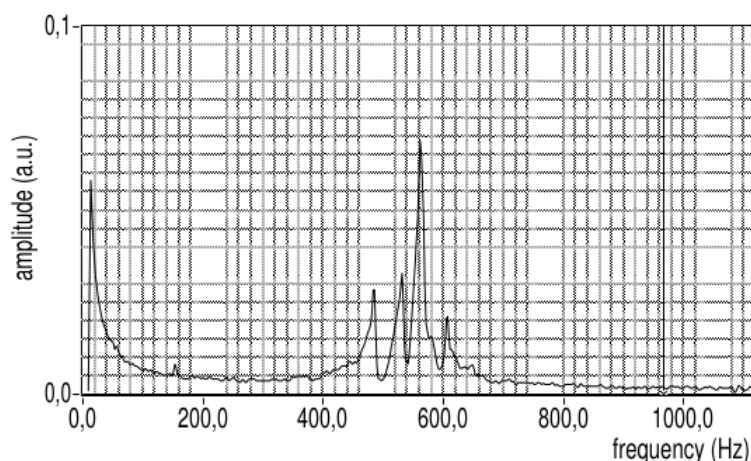
**Figure 3:** *Frequency spectrum of the A+ sample*

| Peak | frequency [Hz] | ppm | difference to TMS | Substance |
|------|----------------|------|-------------------|-----------|
| 1 | 484.0 | 24.4 | 6.2 | $FCH_2$ |
| 2 | 530.0 | 26.8 | 3.8 | $FCH_2$ |
| 3 | 560.0 | 28.3 | 2.3 | $CH_3$ |
| 4 | 606.0 | 30.6 | Reference | |

**Table 2:** *Sample A+*

Sample A is from 2 identified as Fluoroacetone. Fluorine atoms have an odd number of protons and an even number of neutrons in their nucleus such that they posses a nuclear spin of $s = 1/2$, this spin can couple parallely or antiparallely to the proton of the $CH_2$ compound such that we can observe two peaks belonging to $FCH_2$.

| Peak | frequency [Hz] | ppm | difference to TMS | Substance |
|------|----------------|------|-------------------|-----------|
| 1 | 480.0 | 24.2 | 6.9 | Benzene |
| 2 | 574.0 | 29.0 | 2.1 | $CH_3$ |
| 3 | 616.0 | 31.1 | Reference | |

**Table 3:** *Sample B+*

This sample could either correspond to Toluene or to p-Xylene. By comparison with sample E+ we find the intensity of peak 2 in **??** to be much larger than its corresponding value in sample E in **??** such that we identify sample B as p-Xylene.

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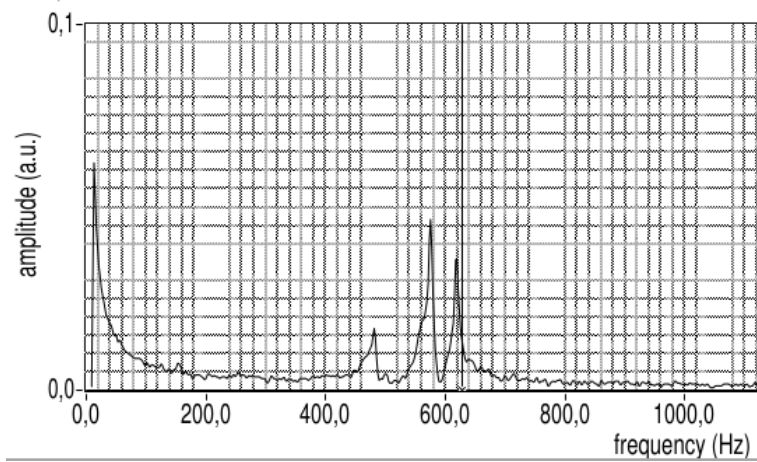
**Figure 4:** *Frequency spectrum of the B+ sample*