

Nuclear magnetic resonance (NMR)

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*All here is
very good*

1 Introduction

With this experiment we research the NMR at the structures of a proton. First of all we test the homogeneity of the permanent magnetic field with a Hall sensor. After that we determine the gyromagnetic ratio γ of a proton (in Glycol and Hydrogen) and the nuclear g-factor of the ^{19}F -atom (in Teflon). For ^{19}F we also determine the magnetic moment.

2 Basics

To determine specific nuclear characteristics we put samples (Teflon, Hydrogen and Glycol) into a high frequency radiation field which is located in a homogeneous magn. field. We use the interaction of the nuclear magn. moment with an external magnetic field to create energy differences (nuclear Zeeman-effect) between two spin stances. When the radiation field frequency reaches the resonance frequency (photon energy equals energy difference), the radiation field loses energy by absorption.

2.1 Nuclear spin

The spin is an intrinsic property of a quantum mechanical particle. Just like the angular momentum, only the absolute value and the projection on a particular axis is determinable:

$$|\vec{S}| = \hbar\sqrt{S(S+1)}, \quad S = 0, \frac{1}{2}, 1, \dots \quad (1)$$

$$S_p = m_S \hbar, \quad -S \leq m_S \leq +S \quad (2)$$

$\hbar \doteq \text{Planck's constant}$

Because the nucleus consists of those particles, it has a spin, too:

$$|\vec{I}| = \hbar\sqrt{I(I+1)} \quad (3)$$

$$I_p = m_I \hbar, \quad -I \leq m_I \leq +I \quad (4)$$

Here you can see that the spin can have $2I+1$ stances.

2.2 Magnetic moment

The spin of a qm particle creates a magnetic dipole moment which interacts with external magnetic fields.

$$\vec{\mu} = \gamma \vec{I}, \quad \text{with } \gamma = \frac{g_I \mu_K}{\hbar} \quad (5)$$

$$\text{with } \mu_K = \frac{e \hbar}{2m_p} \quad (6)$$

$\vec{\mu} \hat{=}$ magn. dipole moment
 $\gamma \hat{=}$ gyromagnetic ratio
 $g \hat{=}$ nucleus g factor
 $e \hat{=}$ elemental charge
 $\mu_K \hat{=}$ nucleus magneton
 $m_p \hat{=}$ proton mass

Because of the 'Pauli Principle' for a nucleus it is only possible to have a spin when there is an odd number of protons or neutrons or both:

$$\begin{aligned}
 ug, gu : I &= \frac{1}{2} \\
 uu : I &= 1 \\
 gg : I &= 0
 \end{aligned}$$

first letter $\hat{=}$ number of protons
second letter $\hat{=}$ number of neutrons
 $g \hat{=}$ even number
 $u \hat{=}$ odd number

Hence Glycol, ^1H and ^{19}F have $I = \frac{1}{2}$.

2.3 Interaction with magnetic and radiation fields (NMR)

A magn. dipole moment $\vec{\mu}$ located in an external magn. field has the energy

$$E = -\vec{\mu} \cdot \vec{B} \quad (7)$$

$$E_p = -g_I \mu_K m_I B_p, \quad (\text{field projection on part. axis}). \quad (8)$$

Two nearby energy levels ($\Delta m_I = \pm 1$) have the energy

$$\Delta E = g_I \mu_K B. \quad (9)$$

This energy is needed or gets free when the spin changes its stance. The energy can be provided by photons (radiation field) with resonance frequency

$$\nu = \frac{\Delta E}{h} = \frac{g_I \mu_K B}{h} = \frac{\gamma B}{2\pi} \quad (10)$$

The proportion of the population number of the two levels ($E_{high} > E_{low}$) in thermal equilibration is given by the Boltzmann distribution

$$\frac{n_{high}}{n_{low}} = e^{-\frac{E_{high}-E_{low}}{kT}} = e^{-\frac{\Delta E}{kT}} \quad (11)$$

$k \hat{=}$ Boltzmann const.

$T \hat{=}$ temperature

\Rightarrow There are more particles in the lower state.

\Rightarrow The radiation field is weakened by absorption.

2.4 Relaxation processes

There are also relaxation processes, which cause a radiationless fall back to the lower level. This keeps the population proportion upright.

2.4.1 Spin-lattice relaxation

Excited nucleuses provide thermal energy to the molecule lattice.

2.4.2 Spin-spin relaxation

The magnetic moment of two particles interact with each other and cause a line broadening and a small shift of the resonance frequency.

2.5 Hall effect and Hall sensor

Moving charge in a conductor is distracted by an external magn. field

$$\vec{F}_L = e (\vec{v} \times \vec{B}) \quad (\text{Lorentz force}) \quad (12)$$

$\vec{v} \hat{=}$ electron drift velocity

This causes a separation of charge until the force of the generated electric field cancels out the Lorentz force ($F_L = F_E$). We can measure the Hall voltage at this field.

$$U_H = vBd = \frac{I}{ne} \quad (13)$$

$d \hat{=}$ conductor width

$I \hat{=}$ current

$n \hat{=}$ charge carrier density

2.6 Lock-In method

The Lock-In measurement method is able to show small signals with a large background noise. The synchron detector multiplies the signal with a reference signal, which has a frequency close to the expected signal. To get a better result for the resonance frequency, we modulate the magnetic field with a saw tooth voltage which is superimposed by a sinus voltage. The generated absorption curve can now be differentially scanned. The zero stands for the minimum of the absorption curve.

3 Measurement methods

3.1 Breadboard

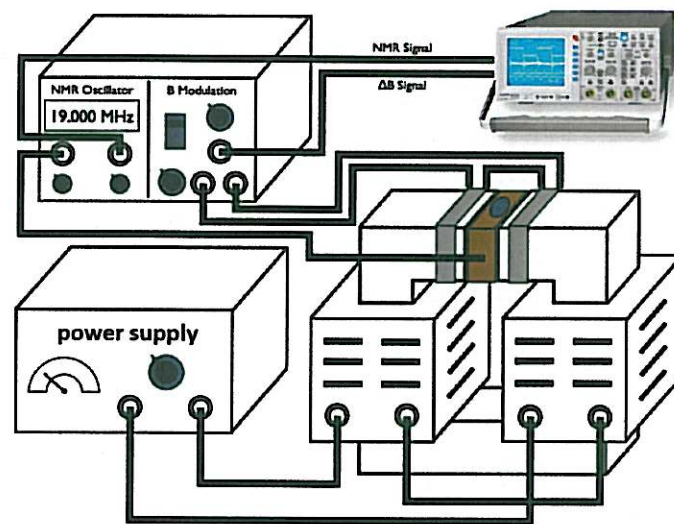


Figure 1: Breadboard for the first measurements

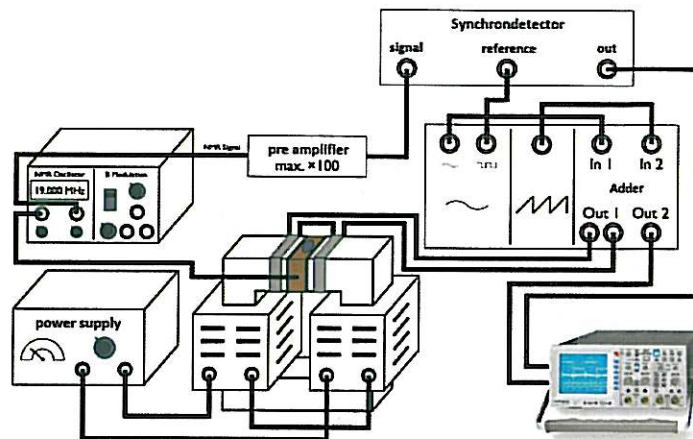


Figure 2: Breadboard for the Lock-in method

The permanent magnetic field is provided by a big electro magnet powered by a power supply. The modulated magnetic field is created by two small coils to the left and the right of the probe holder. They are connected to a sinus voltage at first and an adder at the end. Between the ends of the iron cores of the electro magnet is an electro magnetic oscillating circuit located. There is a hole in the middle of it to put in the Hall sensor or the probes. It is connected to a frequency generator. The oscilloscope is connected to the modulating voltage to show its course. It is also connected to the oscillating circuit to show resonances.

3.2 Experimental procedure

Before the execution of the experiment we had to prove the homogeneity of the magn. field inside the sample holder with a Hall sensor and determine a working point. After that we put a Hydrogen, a Glycol and a Teflon sample inside the field and searched the resonance frequency and measured the magn. field. A sinus modulation of the magn. field made it easier to find and see the absorption signal. At least we adjusted the radiation frequency until the absorption signal matched the modulation zero. So the modulated field strenght was unimportant. To have a better result for Hydrogen, we also used the Lock-in method to measure the time difference between the absorption signal and the magn. field zero for four different frequencies. With a linear regression we could find the resonance frequency.

4 Analysis

4.1 Homogeneity-measurement of the magnetic field with a hall-sensor

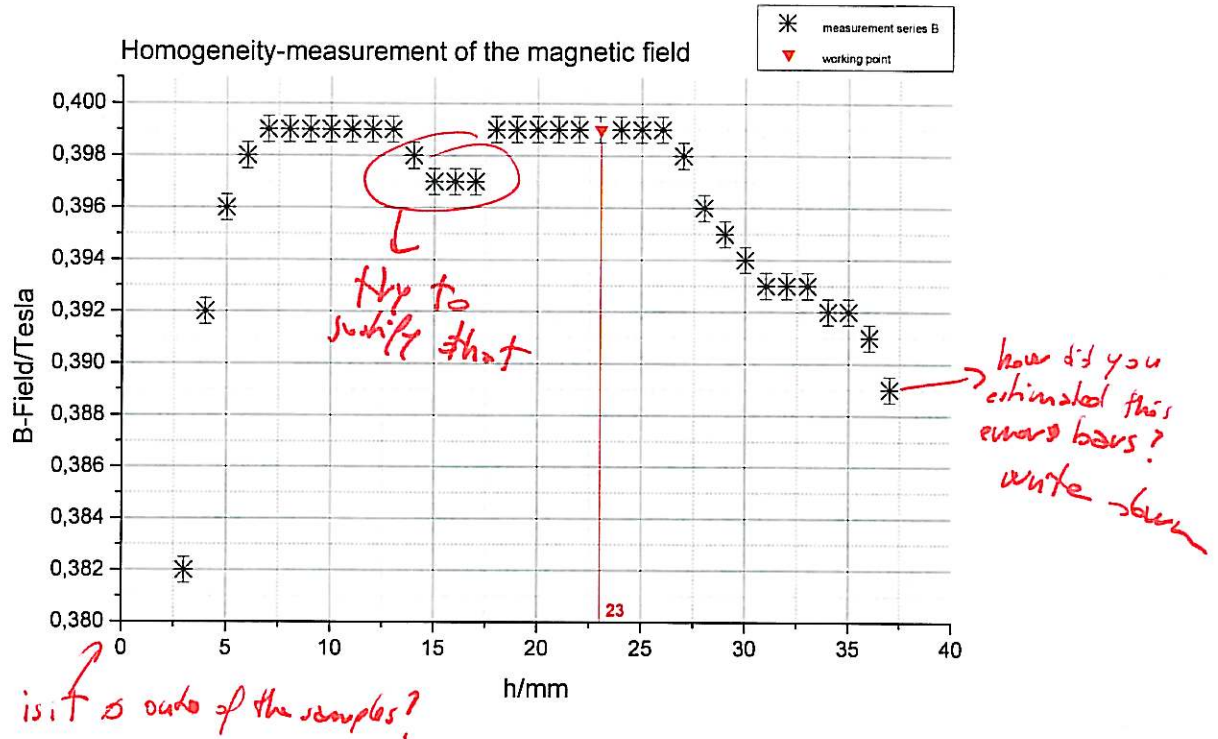


Figure 3: Diagram of the homogeneity-measurement of the magnetic field to find a proper working point

In the diagram above (Figure 3) one can see that there was a inhomogeneous area inside the void where the sample would be placed. This inhomogeneity ranged from 13mm to 18mm. Hence we decided to take (23 ± 1) mm as our working point to guarantee that at least our glycol-samples would not reach the area of the inhomogeneity because the container for the sample was at most filled up to 4mm with glycol. Our direction of the measurement was from 0mm = top to 40mm = bottom of the void. So our working point was around 5mm under the inhomogeneity.

4.2 Nuclear magnetic moment of ^{19}F

Measured values:

$$B = 430 \text{ mT} \pm 0,5 \text{ mT}$$

$$\nu = 17,7578 \text{ MHz} \pm 0,00005 \text{ MHz}$$

→ How is it found

→ How is it estimated?

Nuclear g factor:

$$\begin{aligned} \nu &= \frac{\gamma B}{2\pi} \Rightarrow \gamma = \frac{2\pi\nu}{B} \\ &\Rightarrow \frac{g_F \mu_K}{\hbar} = \frac{2\pi\nu}{B} \\ &\Rightarrow g_F = \frac{\hbar\nu}{\mu_K B} = \frac{4\pi\nu m_p}{eB} \\ &\Rightarrow g_F \approx 5,418 \end{aligned}$$

$$m_p = 1,67262158 \cdot 10^{-27} \text{ kg} \quad (\text{proton mass})$$

$$e = 1,602176462 \cdot 10^{-19} \text{ C} \quad (\text{elemental charge})$$

Calculation of errors:

$$s_{g_F} = \sqrt{\left(\frac{\partial g_F}{\partial B}\right)^2 s_B^2 + \underbrace{\left(\frac{\partial g_F}{\partial \nu}\right)^2 s_\nu^2}_{\text{negligibly small}}} = \frac{\partial g_F}{\partial B} s_B \approx 0,006$$

if introduce symbols write down what is

$$\Rightarrow \boxed{g_F = 5,418 \pm 0,006}$$

$$g_{Lit} = 5,25454 \quad (\text{Handbook of chemistry and physics 1979})$$

Magnetic moment μ_K (with g_{Lit}):

$$\mu_K = \frac{\gamma \hbar}{g_{Lit}} = \frac{\hbar\nu}{g_{Lit} B} \approx 5,208 \cdot 10^{-27} \frac{\text{J}}{\text{T}}$$

$$h = 6,62606876 \cdot 10^{-34} \text{ Js} \quad (\text{Planck's const})$$

$$\hbar = 1,054571596 \cdot 10^{-34} \text{ Js} \quad (\text{reduced Planck's const})$$

Calculation of errors:

$$s_{\mu_K} = \sqrt{\left(\frac{\partial \mu_K}{\partial B}\right)^2 s_B^2 + \underbrace{\left(\frac{\partial \mu_K}{\partial \nu}\right)^2 s_\nu^2}_{\text{negligibly}}} = \frac{\partial \mu_K}{\partial B} s_B = \frac{h\nu}{g_{Lit} B^2} s_B$$

$$\Rightarrow s_{\mu_K} \approx 0,006 \cdot 10^{-27} \frac{J}{T}$$

$$\Rightarrow \boxed{\mu_K = (5,208 \pm 0,006) \cdot 10^{-27} \frac{J}{T}}$$

$$\mu_{Lit} = 5,05 \cdot 10^{-27} \frac{J}{T}$$

4.3 Gyromagnetic ratio of Hydrogen

Measured values:

$$B = 413 \text{ mT} \pm 0,5 \text{ mT}$$

$$\nu = 17,9556 \text{ MHz} \pm 0,00005 \text{ MHz}$$

Gyromagnetic ratio γ :

$$\gamma = \frac{2\pi\nu}{B} = 2,732 \cdot 10^8 \frac{1}{sT}$$

Calculation of errors:

$$s_\gamma = \sqrt{\left(\frac{\partial \gamma}{\partial B}\right)^2 s_B^2 + \underbrace{\left(\frac{\partial \gamma}{\partial \nu}\right)^2 s_\nu^2}_{\text{negligibly}}} = \frac{\partial \gamma}{\partial B} s_B$$

$$\Rightarrow s_\gamma \approx 0,003 \cdot 10^8 \frac{1}{sT}$$

$$\Rightarrow \boxed{\gamma = (2,732 \cdot 10^8 \pm 0,003 \cdot 10^8) \frac{1}{sT}}$$

4.4 Gyromagnetic ratio of Glycol

Measured values:

$$B = 405 \text{ mT} \pm 0,5 \text{ mT}$$

$$\nu = 17,7617 \text{ MHz} \pm 0,00005 \text{ MHz}$$

Gyromagnetic ratio γ :

Calculation analogous to 4.3

$$\gamma \approx 2,756 \cdot 10^8 \frac{1}{sT}$$

Calculation of errors:

Calculation analogous to 4.3

$$s_\gamma \approx 0,003 \cdot 10^8 \frac{1}{sT}$$

$$\Rightarrow \boxed{\gamma = (2,756 \cdot 10^8 \pm 0,003 \cdot 10^8) \frac{1}{sT}}$$

4.5 Measurement of the proton resonance frequency via the Lock-In method

To determine the resonance frequency of the proton, we identified the zero passages of the modulated magnetic field and the signal from the Lock-In amplifier out of the diagrams below (see: section 4.1 diagrams to exercise 5) to get the time difference between both of them to four different frequencies. To obtain the resonance frequency we drew a diagram with the frequencies over the measured time-differences. The y-intercept of a linear fit of the data gives us the resonance frequency. How one can see, it was not easy to find the exact point where the magnetic field passes the x-axis, caused by the sinus-modulation and the resulting width of the Signal - due to that we took the half of the Period as the zero-crossing.

Table: *this table is not readable ~~there~~ try to make a plot like that:*

ν/MHz	18,2873	18,3828	18,4002	18,3401
t_{S1}/s	-3,38	-3,512	-4,744	-5,584
t_{R1}/s	-5,365	-1,776	-1,160	-2,556
t_{S2}/s	7,068	7,112	5,756	5,012
t_{R2}/s	5,16	8,692	9,424	10,892
$\Delta t_1/s$	-1,98	1,736	-3,584	3,028
$\Delta t_2/s$	-1,91	1,58	-3,668	5,880
$S_{\Delta t_1}/s$	$\pm 0,141$	$\pm 0,141$	$\pm 0,141$	$\pm 0,141$
$S_{\Delta t_2}/s$	$\pm 0,141$	$\pm 0,141$	$\pm 0,141$	$\pm 0,141$
$\overline{\Delta t}/s$	1,945	1,658	3,626	4,454
$S_{\overline{\Delta t}}/s$	0,1	0,1	0,1	0,1



$t_R \hat{=}$ time where the absorption – signal crosses the x – axis

$t_S \hat{=}$ time where the magnetic field crosses the x – axis

$$\Delta t_1 = t_{S1} - t_{R1} \quad S_{\Delta t_1} = \sqrt{2} * S_t = S_{\Delta t}$$

$$\Delta t_2 = t_{S2} - t_{R2} \quad S_{\Delta t_2} = \sqrt{2} * S_t = S_{\Delta t}$$

$$\overline{\Delta t} = \frac{1}{N} \sum_{i=1}^N \Delta t_i \quad S_{\overline{\Delta t}} = \frac{S_{\Delta t}}{\sqrt{N}}$$

The failure $S_t = 0,1s$ results from the inaccuracy of reading out the times in the diagrams.

In the table above one can see, that we got strange results for t_{R1} and t_{R2} corresponding to the frequency $\nu = 18,3401$. We assume that these unfitting results were caused by the oscilloscope which probably was half way through with generating a new set of data at the time we read-out the data. So maybe we got a mixture of two data-sets where the time-axis got shifted (see below: Figure 11). Hence, we didnt include these data in our linear regression in the following diagram (Figure 3) and marked them red.

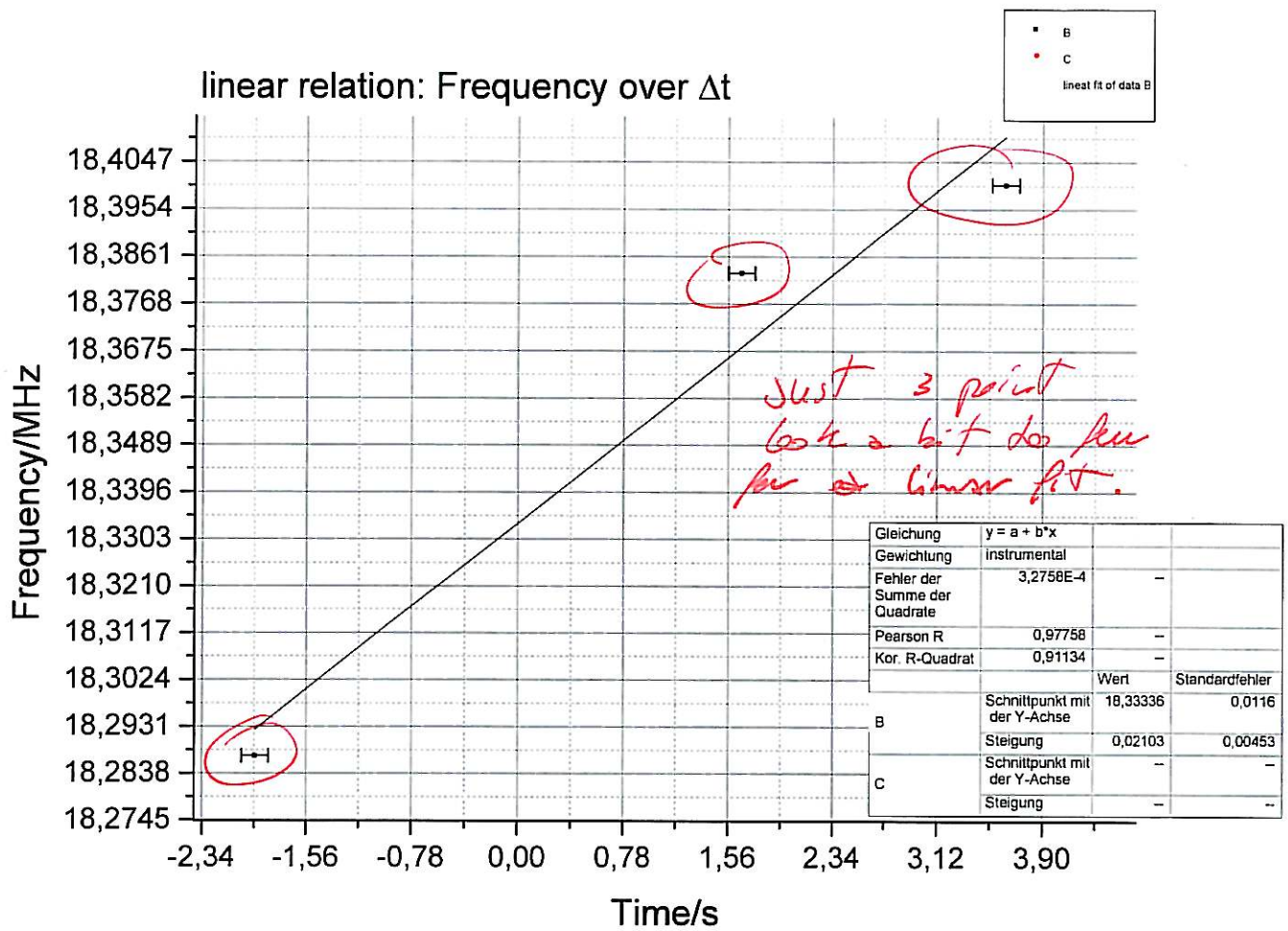


Figure 4: linear regression for the resonancefrequency

The crossing of our linear fit with the y-axis in the diagram above gives us the resonance frequency:

$$\nu_{resonance} = (18,3334 \pm 0,0116)MHz$$

Comparison with the results of 4.2:

Measured values:

$$B = (421 \pm 0,5)mT$$

$$\nu = (18,3334 \pm 0,0116)MHz$$

$$with \gamma = \frac{\nu * 2\pi}{B}$$

$$and s_\gamma = \sqrt{\left(\frac{\partial \gamma}{\partial B}\right)^2 s_B^2 + \left(\frac{\partial \gamma}{\partial \nu}\right)^2 s_\nu^2} \approx 0,0037 * 10^8 \frac{1}{sT}$$

we get $\gamma = (2,7362 \pm 0,0037) * 10^8 \frac{1}{sT}$

This result for the gyromagnetic ratio is in the area of the uncertainties the same as the one we obtained in 4.3

5 Conclusion

In the following sections all results with their literature values are listed and discussed.

5.1 Results for ^{19}F

$$\begin{aligned}g_F &= 5,418 \pm 0,006 \\g_{Lit} &= 5,25454 \\ \mu_K &= (5,208 \pm 0,006) \cdot 10^{-27} \frac{J}{T} \\ \mu_{Lit} &= 5,05 \cdot 10^{-27} \frac{J}{T}\end{aligned}$$

5.2 γ result for Hydrogen

$$\begin{aligned}\gamma &= (2,732 \cdot 10^8 \pm 0,003 \cdot 10^8) \frac{1}{sT} \\ \gamma_{Lit} &= 2,675 \cdot 10^8 \frac{1}{sT}\end{aligned}$$

5.3 γ result for Glycol

$$\begin{aligned}\gamma &= (2,756 \cdot 10^8 \pm 0,003 \cdot 10^8) \frac{1}{sT} \\ \gamma_{Lit} &= 2,675 \cdot 10^8 \frac{1}{sT}\end{aligned}$$

5.4 ν and γ results for Hydrogen with the Lock-In method

Our result for the proton resonance frequency in a magnetic field of 421mT is

$$\begin{aligned}\nu &= (18,3334 \pm 0,0116) MHz \\ \gamma &= (2,7362 \pm 0,0037) * 10^8 \frac{1}{sT} \\ \gamma_{Lit} &= 2,675 \cdot 10^8 \frac{1}{sT}\end{aligned}$$

5.5 Discussion of systematic errors

We can easily see that our results with their uncertainties are not according to the literature value. They are higher. The formulas (in 4.2 – 4.4) show a dependency on the frequency in the numerator and on the magnetic field in the denominator. So this aberration might be caused by a lower actual frequency and/or a higher actual magnetic field. There are some possible reasons for that:

- 1) The first one is our belated magnetic field measurement. We only made notes of the voltage but not of the magnetic field itself at first. So we had to set up the noted voltages again after the experiment to measure the magnetic field. At that time the

old power supply was in operating state for a few hours. It is not unusual that old power supplies lose some voltage over time. So this could have caused a lower magnetic field than we had during our experiment.

- 2) The second one is the observed inhomogeneity from 4.1. That is why the probes were probably affected by a lower magnetic field.
- 3) The third one is an offset change. There might have been a change of external influences on the magnetic field that caused a lowering between our experiment and measurement procedure.

The dimension of a compensating magnetic field increase is about 15mT or a decrease for the frequency is about 0,2 MHz. So it is more realistic that we made a mistake at measuring the magnetic field.

- 4) Another noticeable thing are our uncertainties. There was no information about device specific uncertainties. So we assumed an error about the half of the last display digit. At least the actual hall sensor seems to be bigger.

- 1) If you know that there was this problem, why didn't you repeat the experiment? I think you had time for that or at least to put some statistics about that so to estimate a proper error.
- 2) I think that the errors are under estimated. And also that the "inhomogeneity" should not be there. Did you make (or even try) some test for check that? Did you try to repeat the measurement for get some statistics?

3) I don't put that try to explain better

- 4) Did you ~~also~~ know the difference between "uncertainty" and "error"? If you need the uncertainty of the instruments that are the last digit. But your errors are anyway to small.

If you get a results far from the literature one but with a big error so that they are compatible you are not accurate enough and that could be due to systematic errors or old device, but the experiment is ok.

If you get a results ~~even~~ closer to the literature but out of the error range, you failed the experiment ~~because~~ because you made a wrong analysis and was not able to estimate how good your instruments or procedure are.

You have still the possibility to correct this protocol and to try to make an a posteriori analysis of the results in order to have a better error estimation.

You can add a new chapter where ~~you~~ you explain in details (I do not want that you just multiply the actual value ~~by 10~~) what you did.

(For example you can assume that in fig. 3 between ~ 7 and 27 nm B should be constant and use this data to estimate an error for B)