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A simple and low-cost permanent magnet system for NMR

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ABSTRACT

We have developed a simple, easy to build, and low-cost magnet system for NMR, of which homogeneity is about 4×10^{-4} at 57 mT, with a pair of two commercially available ferrite magnets. This homogeneity corresponds to about 90 Hz spectral resolution at 2.45 MHz of the hydrogen Larmor frequency. The material cost of this NMR magnet system is little more than $100. The components can be printed by a 3D printer.

1. Introduction

Nuclear magnetic resonance (NMR) is one of the most important microscopical probing techniques. There are many applications, such as molecular structure identifications [1], biological sample diagnoses [2], art and culture heritage investigations [3], even demonstrations of quantum computing[4], and quantum artificial intelligence [5]. This powerful technology, however, usually requires large space, huge cost and complicated maintenance. Therefore, only a few students and researchers have an opportunity to employ it.

Recently, small magnets based on the Halbach design [6], therefore compact NMR spectrometers, have been reported [7–21]. Although they are simpler and more compact than conventional high resolution NMR spectrometers, they are not yet simple or low cost enough for educational purposes.

In this manuscript, we present a significantly simple NMR magnet system composed of a pair of two commercially available, and thus affordable, ferrite magnets which are facing with each other. The non-fidelity of the magnetization distribution of individual ferrite magnets is significantly large and thus we compensate them by inserting a pair of two thick magnetically soft discs in-between. Despite of this simple design, the homogeneity of 4×10^{-4} is obtained at 57 mT (or, an about 90 Hz spectral resolution at the 2.45 MHz hydrogen Larmor frequency). This is adequate to perform basic and educational NMR experiments, such as T_1 and T_2 measurements.

2. NMR magnet system design

We employ a pair of two commercially available [22] ferrite magnets to make our NMR magnet system affordable. Then, we put two magnetically soft (pure iron [23]) discs in-between in order to obtain as good as possible homogeneity. Our NMR magnet system is not only affordable but also significantly simple, as shown in Fig. 1.

2.1. Surface fields of ferrite magnets

We first characterize twelve Y30BH ferrite magnets of disk shape [22] of which diameters are 120 mm and thicknesses are 20 mm. We measure magnetic fields at 1.6 mm above the north surfaces of them with a calibrated hall device. The measurements are performed by carefully removing any magnetic materials near the objects under investigation. The intervals between measured points are 5 mm and the total measured points are 421 points, as shown in Fig. 2. Hereafter, we call these measured magnetic fields as the surface fields. They are not perfectly axisymmetric. The north and south sides are not symmetric, either.

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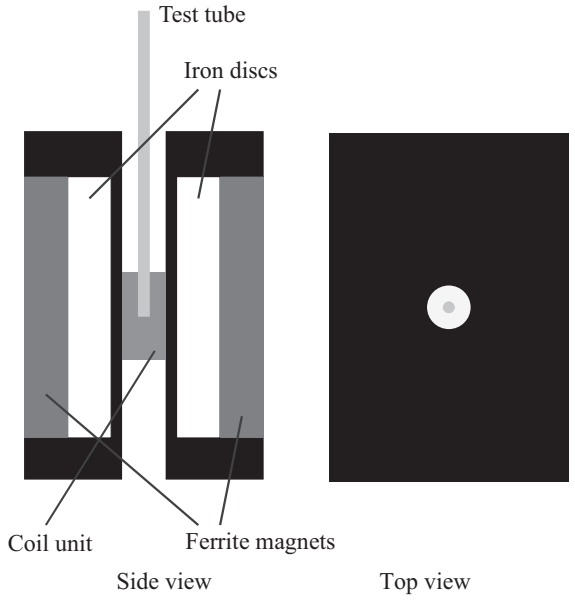

Fig. 1. Sketch of our NMR magnet system. The black part is a magnet base on which the ferrite magnets and iron discs are set with their magnetic attractive forces. The coil unit contains the pickup and saddle coil.

2.2. NMR magnet system

We make a base which is schematically shown in Fig. 1. We first put only matched pair of ferrite magnets on it. The distance between them is 30 mm. Because of the attractive force between them, it is not necessary to fix them with a specific fixture. This base can be constructed by machining a bulk material, such as acrylic, as shown in Fig. 3. Its total (material and machining) cost was about $400. On the other hand, it can also be printed with a 3D printer, as shown in Fig. 4. In this case, it is necessary to finish it by machining so that the central part is parallel and flat. The cost of ABS filament for printing is less than $20. We obtain a field of about 85 mT and a reasonably good field homogeneity of 3300 ppm, see Section 3.2. We can perform NMR measurements with it.

Then, we put a pair of two iron discs between these two magnets in order to obtain higher homogeneity. Although the flux shaping effect of iron discs, or pole pieces, might be well-known, we show Fig. 5 in order to justify our approach. The results are discussed in detail in Section 3. The NMR magnet system, shown in Fig. 4, is about 110 mm × 140 mm × 120 mm and weighs about 7 kg.

We purchased 12 ferrite magnets and so far found 2 pairs of magnets that can be employed to build the NMR magnet system. Each ferrite magnet costs only $16. Therefore, the cost of ferrite magnets is less than $100 per one NMR magnet system in the worst case. If we make more NMR magnet systems, the cost of ferrite magnets for each NMR magnet system should approach $16 ×2. On the other hand, a pure iron disk costs $25/disc [23]. Its surface must be smooth but this is achieved by machining with a lathe. This surface treatment does not cost very much.

3. Measurements

We measure several NMR spectra in order to evaluate our NMR magnet systems. We mainly show the results with Nos. 4 and 5 ferrite magnets.

3.1. Coil system and electronics

The pickup coil, of which length is 3 mm (or 5 mm) is wound on a standard 3 mm (or 5 mm) NMR test tube and then casted with stycast 1266 [26] in the bobbin printed by a 3D printer, as shown in Fig. 4. The saddle coil is done 20 times on the bobbin. The resistance and inductance of the pickup coil are typically 4.2 Ω (0.8 Ω) and 27 μH (8.9 μH) for a 3 mm (5 mm) NMR test tube, respectively. Those of the saddle coil are typically 6.1 Ω and 25 μH, respectively.

We employ an arbitrary wave function generator (WF1974: NF Circuit Design) as a pulse generator and a RF power amp. RF pulses are fed to the saddle coil through a matching circuit. The signal from the pickup coil is amplified by a low noise preamp. (CA-251F4: NF Circuit Design) and directly measured with an oscilloscope (MOD3012: Tektronix) without converting the frequency.

3.2. Homogeneity

The field homogeneity of our NMR magnet is evaluated by hydrogen spectra measured with water in a standard 3 mm (or 5 mm) NMR test tube [25]. The water contains magnetic impurity of $CuSO_4$ in order to shorten T_1. 512 FID signals measured in 2 min are averaged and then a spectrum is calculated.

The FWHM of the spectrum obtained without pure iron discs is 3.4 kHz with a 3 mm NMR test tube (11.5 kHz with a 5 mm NMR test tube) at the Larmor frequency of 3.5 MHz (85 mT), as shown in the left panel of Fig. 6. It corresponds to about 1000 ppm (3300 ppm) homogeneity.

The FWHM of the spectrum obtained with the pure iron discs is 90 Hz with a 3 mm NMR test tube (230 Hz with a 5 mm NMR test tube) at the Larmor frequency of 2.45 MHz (57 mT), as shown in the right panel of Fig. 6. It corresponds to 35 ppm homogeneity. We can also obtain a similar homogeneity with Nos. 7 and 8 ferrite magnets although the Larmor frequency becomes slightly smaller (2.43 MHz). The iron discs improve homogeneity as expected.

It is interesting to note that the directions of the ferrite magnets around their axes should be adjusted to obtain the best homogeneity, as reported in Ref. [17]. Table 1 summarizes the measured FWHM as a function of the relative rotation angle between Nos. 4 and 5 magnets.

3.3. T_1 and T_2 Measurements

Typical T_1 and T_2 measurements of a water sample without magnetic impurities are shown in Fig. 7. T_1 is measured by the inversion recovery method, while T_2 is measured by the spin echo experiments.

3.4. Scalar coupling constant measurements

The spectra of hydrogen (H) and carbon-13 (^{13}C) of ^{13}enriched chloroform are measured, as shown in Fig. 8. Two peaks in the spectra are clearly observed for both H and ^{13}C although the signal of ^{13}C is smaller than that of H.

512 FID signals are averaged in 2 min in order to obtain the above spectra. The drift of the field due to temperature changes may degrade the spectra as discussed in Ref. [8]. This drift may be more serious in our case than theirs because the temperature coefficient of ferrite magnet magnetization is −0.5%/K and larger than that of SmCo of −0.035%/K [15]. It may be better to perform

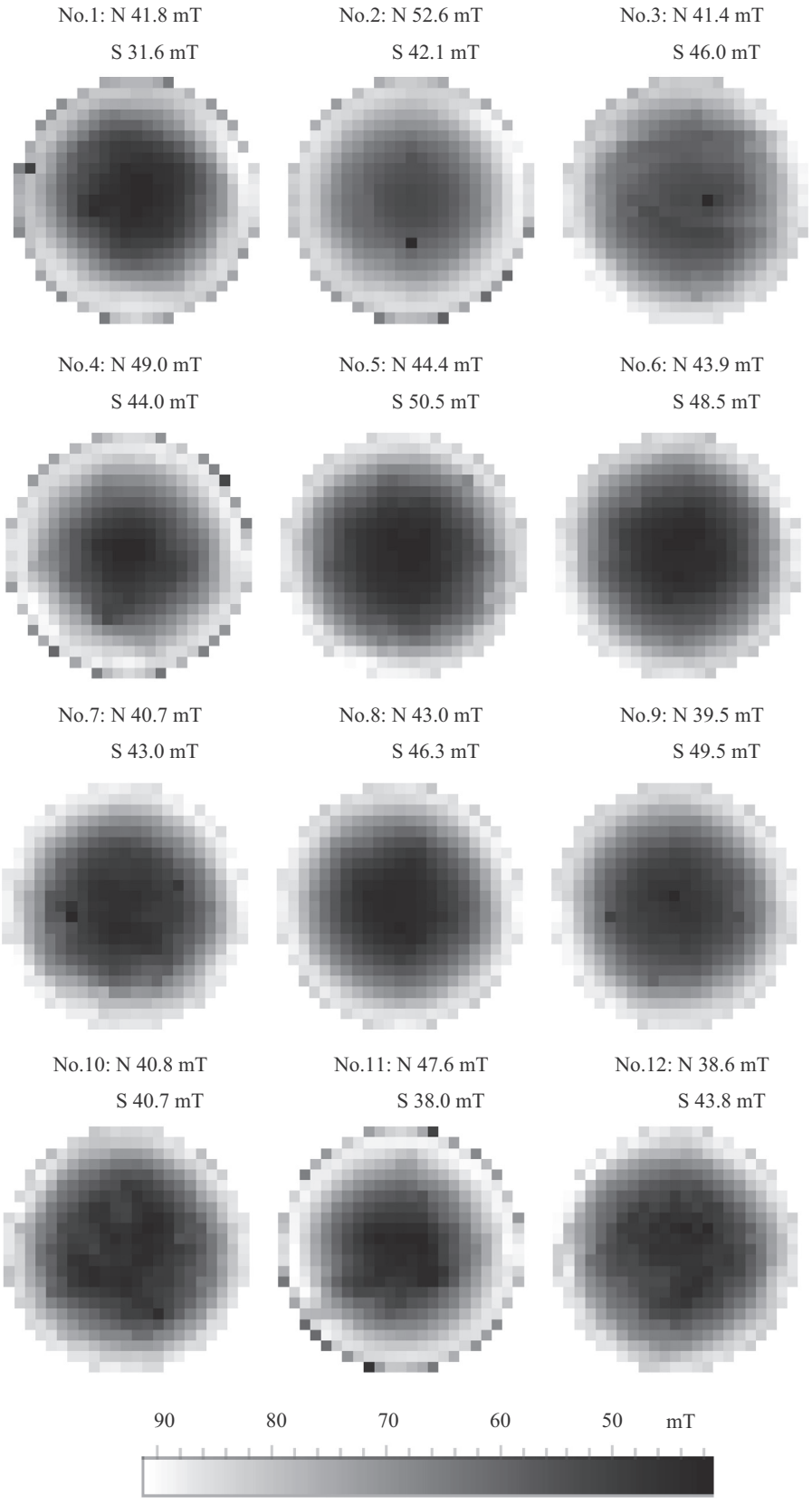

Fig. 2. Measured fields at 1.6 mm above the surfaces of the north sides of twelve ferrite magnets. The intervals between measured points are 5 mm. The magnetic fields at the center of both the north and south sides are shown, as well. The fields of the south sides are measured only at the centers.

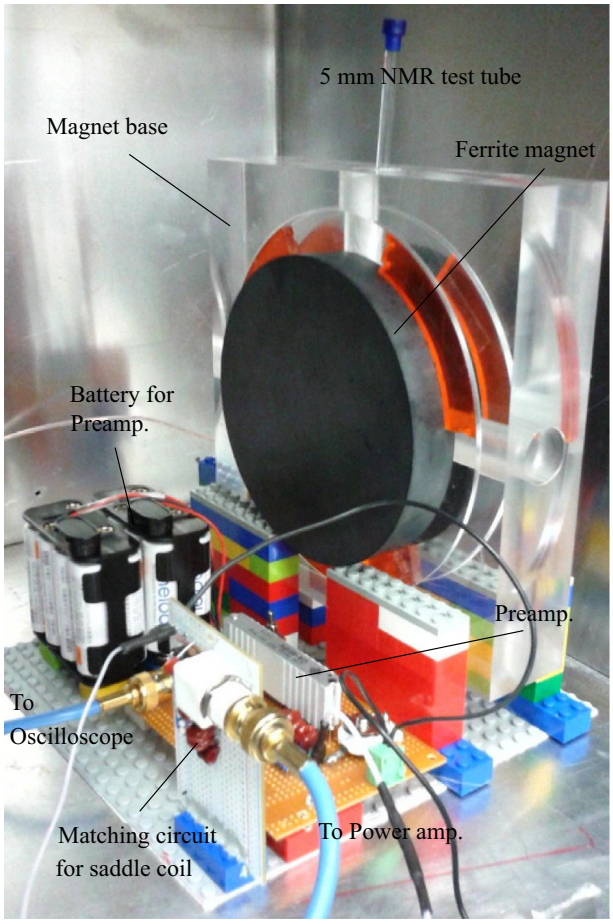

Fig. 3. The magnet system made of acrylic and electronics for measurements.

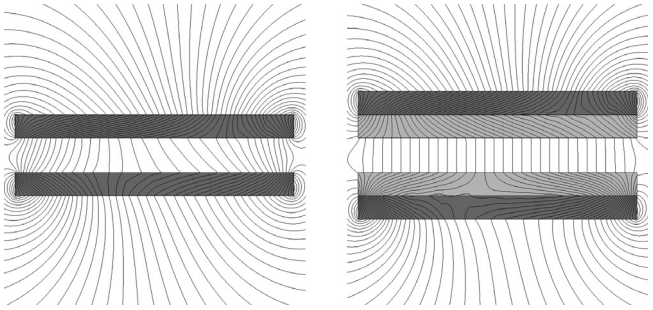

Fig. 5. Iron disks can homogenize a field. Sketches of flux lines with (the right panel) and without (the left panel) iron discs (gray discs) are shown. These are simulations calculated with FEMM [24].

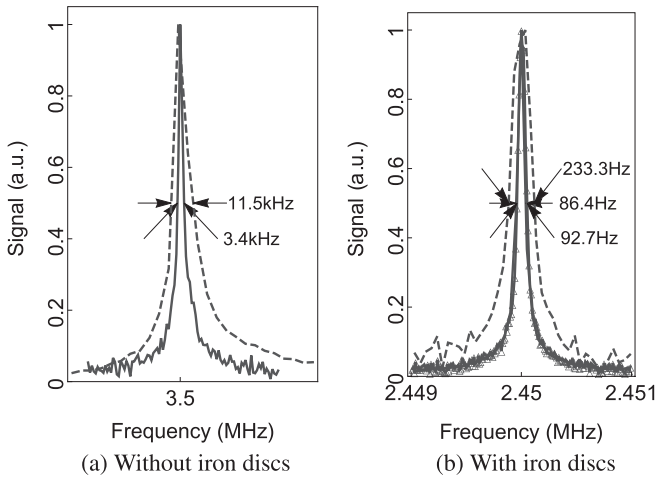

Fig. 6. (a) Hydrogen spectra of doped water with a 5 mm (dashed) and 3 mm (thick) NMR test tube without iron discs and (b) ones with a 5 mm (dashed) and 3 mm (thick) NMR test tube. Nos. 4 and 5 ferrite magnets are selected. △'s are obtained when Nos. 7 and 8 ferrite magnets are employed. Note that △'s are shifted from 2.43 MHz for comparison.

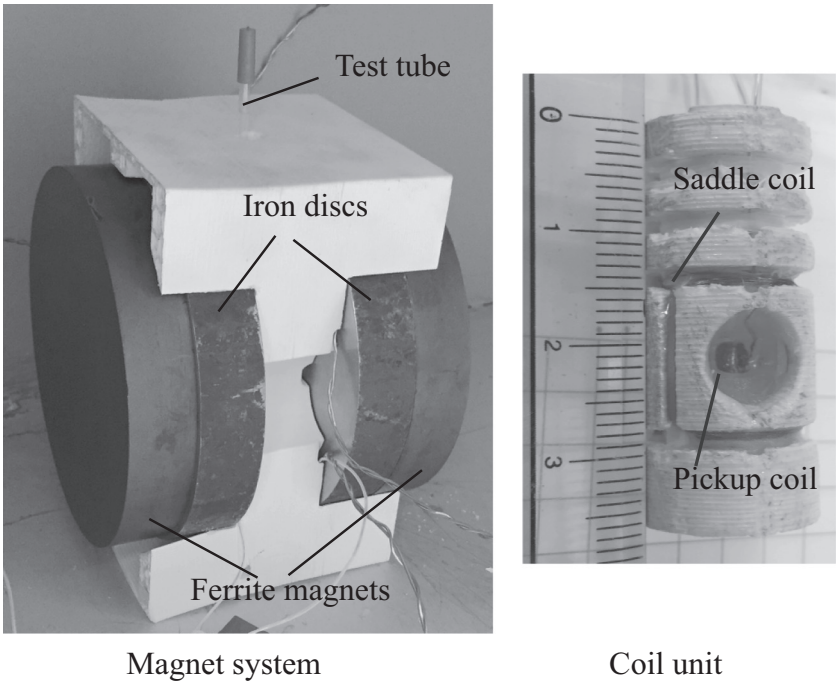

Fig. 4. The white magnet base is monolithic and printed by a 3D printer. The magnet system is placed in a styrene foam box in order to stabilize its temperature. It does not require extra electric shields. The coil unit contains the pickup and saddle coils and is placed in the center of the magnet system, as shown in Fig. 1. The coil bobbin is also printed.

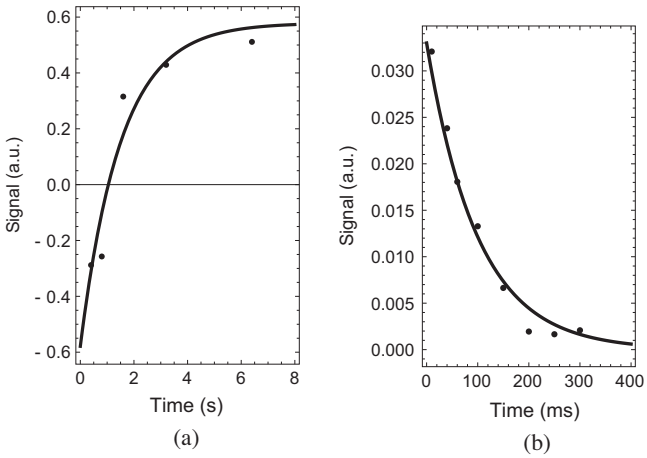

Fig. 7. Typical (a) T_1 and (b) T_2 measurements of the water sample.

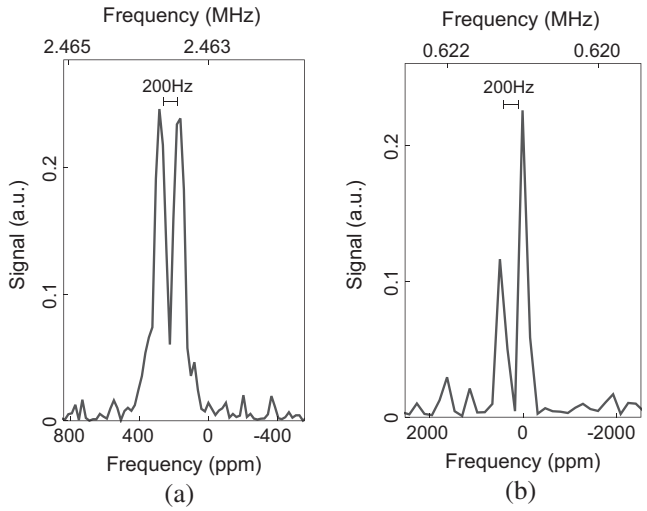

Fig. 8. Spectra of chloroform. (a) H and (b) ^{13}C spectra are measured with our NMR magnet system. The scalar coupling constant between H and ^{13}C is measured to be 215 Hz with a commercial NMR spectrometer (ECA500, JEOL Resonance) at 11.75 T.

a long-term averaging by frequency-shifting individual spectrum before summing [8] in the case of ^{13}C measurements.

3.5. Chemical shift measurements

It turns out that our magnet system is adequate to observe a chemical shift if a proper molecule, such as 3 chloro-2,3,4,5,6 tetrafluoro-benzo-trifluoride (the upper right panel of Fig. 9), is selected.

The spectrum of ^{19}F in 3 chloro-2,3,4,5,6 tetrafluoro-benzo-trifluoride is shown in the upper left panel of Fig. 9. Two peaks are observed. The higher frequency peak corresponds to F in $-CF_3$, while the lower one corresponds to F's attached on the Benzene ring. The differences among F's attached on the Benzene ring cannot be seen. The difference between these two peaks is about 90 ppm and in good agreement with the measured one with a commercial NMR spectrometer (ECA-500, JEOL Resonance) at 11.75 T, as shown in the lower panel of Fig. 9.

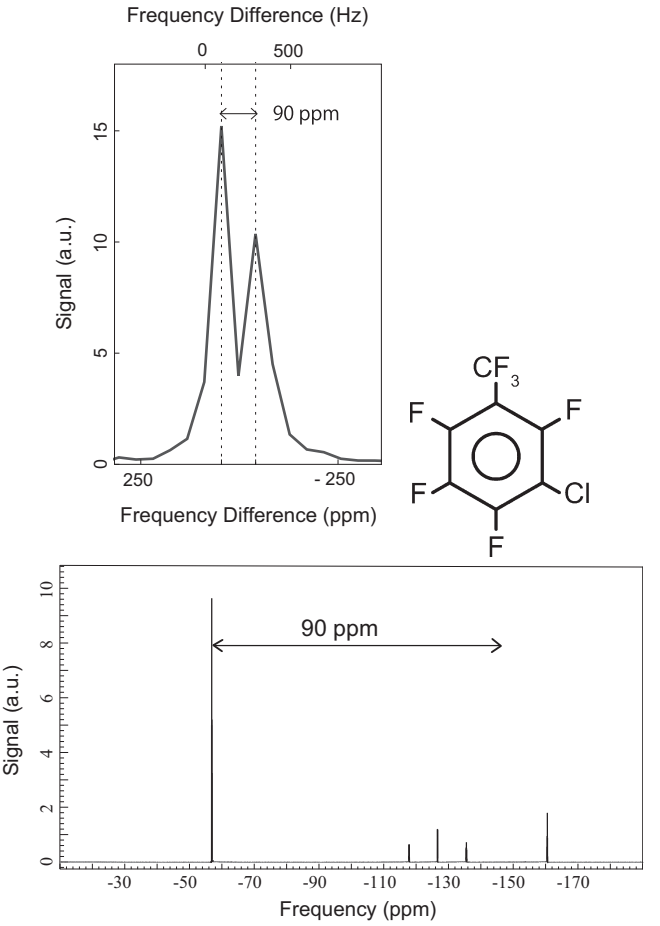

Fig. 9. Spectra of ^{19}F in 3 chloro-2,4,5,6 tetrafluoro-benzo-trifluoride. The upper left panel shows a spectrum measured with our magnet, while the lower panel with a commercial NMR spectrometer (ECA-500, JEOL Resonance) at 11.75 T. The upper right panel is a structure of this molecule.

Table 1
FWHM's of hydrogen spectra of doped water measured with a 3 mm NMR test tube as a function of the relative rotation angle between Nos. 4 and 5 ferrite magnets.

θ (°)	Δf (Hz)	θ (°)	Δf (Hz)
30	338.0	210	296.0
60	329.3	240	116.0
90	394.7	270	259.8
120	272.7	300	273.5
150	296.4	330	236.0
180	296.8	360	285.4

4. Conclusions

We have developed a simple, easy-to-build, and low-cost NMR magnet system with a pair of two commercial ferrite magnets. The field homogeneity is improved by inserting a pair of two iron discs between them. A 90 Hz frequency resolution in spectra at about 2.4 MHz Larmor frequency is obtained. Moreover, the standard NMR measurements, such as chemical shifts, scalar couplings, T_1's, and T_2's, can be performed and thus our NMR magnet system is suitable for educational purposes because of its simplicity, affordability, and reasonably good field homogeneity.

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