Hyperfine field and hyperfine anomalies of copper impurities in iron

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A new value for the hyperfine magnetic field of copper impurities in iron is obtained by combining resonance frequencies from experiments involving β-NMR on oriented nuclei on ^{59}Cu, ^{69}Cu, and ^{71}Cu with magnetic moment values from collinear laser spectroscopy measurements on these isotopes. The resulting value, i.e., $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.794(10)$ T, is in agreement with the value adopted until now but is an order of magnitude more precise. It is consistent with predictions from *ab initio* calculations. Comparing the hyperfine field values obtained for the individual isotopes, the hyperfine anomalies in Fe were determined to be $^{59}\Delta^{69} = 0.15(9)\%$ and $^{71}\Delta^{69} = 0.07(11)\%$.

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I. INTRODUCTION

Precise values of magnetic hyperfine fields [1] allow the determination of nuclear magnetic moments by experimental methods such as integral perturbed angular correlation [2] and time-differential perturbed angular distribution [3], or low-temperature nuclear orientation (LTNO) and nuclear magnetic resonance on oriented nuclei (NMR/ON) [4]. Precise results, in addition, allow a detailed comparison with theory.

The magnetic hyperfine fields of substitutional impurities in bcc Fe are at present well understood for most of the elements in the Periodic Table [5–11], with sizable differences between theory and experiment remaining mainly for the heavier 5*d* impurities [12,13], the alkaline elements [14–17], and the actinides [11]. Still, for a few elements no precise experimental results are available yet. A special case is copper, for which the currently accepted value of the hyperfine field in iron is $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.8(1)$ T [18]. This value resulted from a spin-echo NMR measurement with the sample containing the stable isotopes ^{63}Cu and ^{65}Cu cooled to a temperature of 4.2 K. The error of 0.1 T was not given in the original publication but was provided later as a private communication by one of the original authors [19]. The sign was obtained from the field shift in NMR measurements [20] and was confirmed by theoretical calculations (Ref. [21] and Sec. VI).

In the past few years the magnetic hyperfine interaction frequencies $\nu_{\mathrm{res}} \sim \mu B_{\mathrm{tot}}$, with μ the nuclear magnetic moment and B_{tot} the total magnetic field the nuclei experience, have been determined for the Cu isotopes ^{59}Cu [22], ^{67}Cu [19], ^{69}Cu [23], and ^{71}Cu [24] with the β-NMR/ON method, i.e., NMR/ON with β-particle detection. In these measurements, performed on samples that were cooled to millidegree Kelvin temperatures, the aforementioned value for the hyperfine field of Cu impurities in the Fe host, viz., $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.8(1)$ T, was used to extract the nuclear magnetic moments for the isotopes studied. Recently, the magnetic moments of the Cu isotopes with $A = 61$ to 75, i.e., including the ones mentioned earlier, were determined by collinear laser spectroscopy measurements at the Isotope Separator On Line facility at CERN (ISOLDE-CERN) [25–27]. Because results for the β-NMR/ON resonance frequencies and for the magnetic moments from the laser spectroscopy measurements for these isotopes all have similarly high precisions, ranging from 2×10^{-4} to 6×10^{-4}, combining these results allows a new and precise value to be determined for the hyperfine magnetic field of Cu in Fe at 0 K.

Note that the resonance frequencies and magnetic moment values that are used here were all obtained with the same experimental methods and setups. This reduces the risk for possible systematic errors related to calibration issues.

II. NUCLEAR MAGNETIC RESONANCE ON ORIENTED NUCLEI

The NMR/ON method has been applied widely for the precise determination of the magnetic hyperfine splitting of radioactive nuclei in the ferromagnetic host lattices Fe, Co, and Ni. In most cases, the primary goal was to deduce the nuclear magnetic moments of the impurity isotopes [28]. The same technique is also used to study ground state spins [29], hyperfine fields [1,30], nuclear relaxation times [31,32], and quadrupole splittings [33,34], as well as to obtain information on the lattice location and implantation behavior of implanted impurities [13,35–37]. NMR/ON experiments require the nuclei to be oriented, which is done using the LTNO method [4] and requires cooling down the radioactive samples to temperatures in the millidegrees Kelvin region and subjecting them to high magnetic fields, either hyperfine magnetic fields [4] or externally applied fields [38].

In NMR/ON, the resonant depolarization of the radioactive probe nuclei is detected as a function of the frequency of the applied radio-frequency field via the resulting destruction of

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anisotropy in the anisotropic emission of the decay radiation. The resonance frequency is related to the hyperfine field, B_{hf}, through the relation

$$\nu_{\text{res}}[\text{MHz}] = \left| \frac{7.6226\mu[\mu_{\text{N}}]B_{\text{tot}}[\text{Tesla}]}{I[\hbar]} \right| \tag{1}$$

with I the nuclear spin of the isotope studied and

$$B_{\text{tot}} = B_{\text{hf}} + B_{\text{app}}(1 + K) - B_{\text{dem}}. \tag{2}$$

Here the hyperfine field B_{hf} includes the Lorentz field of 0.742 T for bcc iron at 0 K, B_{app} is the externally applied magnetic field, B_{dem} is the demagnetization field, and K is the Knight shift. The constant factor is the ratio of the fundamental constants μ_N/h and it does not contribute to the error budgets here.

III. COLLINEAR LASER SPECTROSCOPY

Collinear laser spectroscopy experiments determine the hyperfine structure of atomic ground and excited states, yielding precise values for the hyperfine parameters A and B, which in turn provide accurate values for magnetic and quadrupole moments of the isotopes studied [39].

Recently, collinear laser spectroscopy experiments were performed on a series of Cu isotopes at ISOLDE with the COLlinear LAser SPectroscopy (COLLAPS) setup, including the four isotopes for which resonance frequencies are available from recent β-NMR/ON measurements. For several of these isotopes, laser spectroscopy could only be performed after the installation of the ISolde COOLer (ISCOOL) cooler and buncher radio-frequency quadrupole Paul trap [40,41]. This allowed the collinear laser setup to be operated in bunched mode, reducing the background photon counts from scattered laser light by more than three orders of magnitude and permitting measurements to be made on isotopes that were previously not accessible due to their low yields. The Cu^+ bunches from ISCOOL were sent through a sodium vapor cell, which neutralized the ions through charge-exchange collisions. A voltage was applied to the vapor cell for tuning the velocity of the ions and bringing them into resonance with the laser beam that was overlapped with the Cu beam in the co-propagating direction. Resonances were located by measuring the photon yield as a function of the voltage with two photomultiplier tubes, the voltage of which was gated so that photons were only recorded when an atom bunch was within the light-collection region [25]. An example of a collinear resonance fluorescence spectrum obtained in these measurements is shown in Fig. 1 of Ref. [25].

IV. HYPERFINE MAGNETIC FIELD FOR COPPER IN IRON

In the following, the magnetic moments from the collinear laser spectroscopy measurements on the isotopes ^{59}Cu [27], ^{67}Cu [26], ^{69}Cu [26], and ^{71}Cu [25] are combined with the β-NMR/ON measurements that were performed on these isotopes [19,22–24]. The experimental magnetic moment values and β-NMR/ON resonance frequencies for ^{59}Cu, ^{69}Cu, and ^{71}Cu are listed in Table I and are discussed in Sec. IV B. The data for ^{67}Cu are discussed separately in Sec. IV C.

Because the extraction of the hyperfine magnetic field using Eqs. (1) and (2) requires that a possible Knight shift and the demagnetization field are taken into account as well, the β-NMR/ON measurements and these two factors are addressed in some detail first.

A. β-NMR/ON measurements

All four Cu isotopes on which β-NMR/ON measurements were produced at the ISOLDE isotope separator facility. The NMR/ON measurements were performed either on-line using the Nuclear Implantation into Cold On Line Equipment (NICOLE) LTNO setup [44] at ISOLDE (for ^{59}Cu [22], ^{69}Cu [23], and ^{71}Cu [24]), or off-line with the nuclear-orientation facility at Oxford University (for ^{67}Cu [19]). As an example, the NMR/ON result for ^{59}CuFe is shown in Fig. 1.

1. Demagnetization field

The calculation of the demagnetization field is not straightforward, but for the simple shapes and thin foils (magnetized in the plane of the foil) that were used in the β-NMR/ON measurements discussed here, analytical expressions can be obtained [43]. At the current level of precision, the small

TABLE I. Data used for the determination of the hyperfine field of Cu impurities in Fe and values deduced from these data. The error bar on the weighted average was increased by a factor of $\sqrt{\chi^2/\nu} = \sqrt{1.22}$ to account for the fact that the reduced χ^2 is larger than unity. The last column lists the hyperfine anomaly differences between ^{69}Cu and the two other isotopes.

Isotope	μ (μ_N)	Ref.	ν_{res} (MHz)	Ref.	B_{tot}[a] (T)	B_{app}[b] (T)	B_{dem} (T)	B_{hf}[a] (T)	$^{X}\Delta^{69}$ (%)
^{59}Cu	+1.8910(9)	[27]	208.79(4)	[22]	−21.727(11)	0.100(5)	0.020(4)[c]	−21.807(13)	0.15(9)
^{69}Cu	+2.8383(10)	[26]	311.7(1)	[23]	−21.611(10)	0.20(1)	0.036(8)[c]	−21.775(16)	
^{71}Cu	+2.2747(8)	[25]	250.00(14)	[24]	−21.627(14)	0.20(1)	0.036(8)[c]	−21.791(19)	0.07(11)
Weighted average								−21.794(10)	

[a] Sign from Ref. [42].

[b] From the references listed in column 5.

[c] Calculated with the formulas derived in Ref. [43] (see also Sec. IV A1).

demagnetization fields in the foils used, which are of the order of 0.01 T, cannot be neglected.

The foil used by the Leuven group for the measurement with ^{59}Cu had a size of 9 mm by 14 mm and an initial thickness of 125 μm. It was polished with diamond-base paste with grain sizes of 3 and 1 μm. It is estimated that this reduced the thickness of the foil to 95 ± 20 μm. For this a demagnetization field $B_{\text{dem}} = 0.020(4)$ T is calculated. The foils used by the Oxford group for the measurements with ^{67}Cu, ^{69}Cu, and ^{71}Cu had an initial thickness of 250 μm [45]. They were first polished with sandpaper with CAMI (Coated Abrasive Manufacturers Institute) grit designation 600 (i.e., with an average particle diameter of 16 μm) and thereafter also with diamond-base paste. Owing to the larger particle diameter used in the first step, this procedure removed more material from the foils, leading to an estimated thickness of 190 ± 40 μm. For typical dimensions of 10 mm by 15 mm for such foils, a demagnetization field $B_{\text{dem}} = 0.036(8)$ T is then calculated for the measurements with ^{67}Cu, ^{69}Cu, and ^{71}Cu.

2. *Knight shift*

The Knight shift for copper in iron has never been determined at low temperatures. For other elements in ferromagnetic host materials, Knight shift values ranging from zero to about 5% have been reported [46]. Thus, for the low external fields, B_{app}, of 0.1 and 0.2 T that were used in the β-NMR/ON measurements discussed here, the Knight shift corrections could amount up to about 0.005 and 0.010 T, respectively. These values were then used as the 1σ error bars on the values for the externally applied magnetic fields. Note that the precision to which these external fields could be set is an order of magnitude better and can therefore be neglected at the current level of precision.

B. Results for ^{59}Cu, ^{69}Cu, and ^{71}Cu

The magnetic moment values and the resonance frequencies for the isotopes ^{59}Cu, ^{69}Cu, and ^{71}Cu are listed in Table I (the case of ^{67}Cu is discussed separately in the next section). Also listed in Table I are the values for the total magnetic field, B_{tot}, obtained for each isotope using Eq. (1), as well as the hyperfine field, B_{hf}, that is then obtained from Eq. (2) using the values for the externally applied field, B_{app}, and the demagnetization field, B_{dem}.

As can be seen, the hyperfine field values obtained for these three isotopes are in very good agreement with each other (see also Fig. 2). Combining all three results yields a weighted-average value of

$$B_{\text{hf}}(\text{CuFe}) = -21.794(10)\ \text{T}. \tag{3}$$

The differences between the hyperfine field values obtained for the three isotopes listed in Table I could be due to small differences in the distribution of the nuclear magnetization over the nuclear volume for the three isotopes, i.e., hyperfine anomalies [47]. The usual definition for the hyperfine anomaly, ϵ_i, for a single nuclear state i is

$$B_{\text{eff}} = B_0(1 + \epsilon_i), \tag{4}$$

where B_{eff} is the hyperfine field averaged over the distribution of nuclear magnetization of the state i and B_0 is the hyperfine field at $r = 0$. The difference of the hyperfine anomalies of two nuclear states in the same host metal is then given by

$$^1\Delta^2 = \epsilon_1 - \epsilon_2 = \frac{B^1_{\text{eff}}}{B^2_{\text{eff}}} - 1. \tag{5}$$

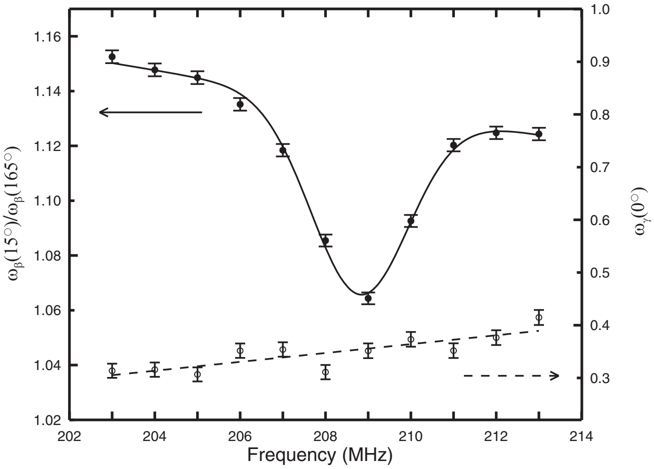

FIG. 1. On-line NMR/ON curve for ^{59}Cu isotope. Plotted is the ratio of the count rates for two detectors at 15° and 165° with respect to the quantization axis as a function of frequency. At the bottom, the count rate at 0° is shown for the 136-keV γ ray of the ^{57}CoFe thermometer (corresponding to a sample temperature of about 10 mK) for the same frequency region, showing no effect at the position of the ^{59}Cu resonance. The slope in the count rates is caused by a small increase of the sample temperature with the resonance frequency. (Arrows indicate the vertical scale that applies; from Ref. [22].)

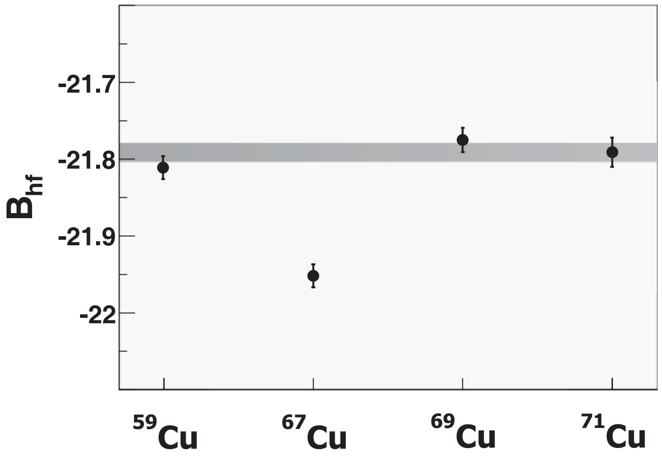

FIG. 2. Hyperfine field values (in Tesla) for Cu in Fe obtained by combining resonance frequencies from β-NMR/ON measurements on the isotopes ^{59}Cu, ^{67}Cu, ^{69}Cu, and ^{71}Cu with the magnetic moments for these isotopes from collinear laser spectroscopy. The shaded band indicates the weighted average of the values from ^{59}Cu, ^{69}Cu, and ^{71}Cu.

When considering the possible presence of hyperfine anomalies the values for B_{hf} listed in Table I have to be interpreted as values for B_{eff}. It then turns out that the differences of the hyperfine anomalies of these three isotopes are less than 3×10^{-3} (see Table I; 90% C.L.). Note that previously the hyperfine anomaly between ^{63}Cu and ^{65}Cu was estimated to be less than 5×10^{-5} [48]; in the recent collinear laser spectroscopy measurements on Cu isotopes [26], no indication for hyperfine anomalies was observed either for the series of isotopes ranging from $A = 61$ to 75.

For ^{59}Cu, two other values for the magnetic moment were recently quoted as well, i.e., $\mu(^{59}\mathrm{Cu}) = 1.83(4)\mu_N$, from in-source laser spectroscopy [49], and $\mu(^{59}\mathrm{Cu}) = 1.910(4)\mu_N$, from an in-gas-cell laser spectroscopy experiment [50,51]. Because the first value is much less precise than the one obtained from collinear laser spectroscopy, it is not further used here. The second value differs well outside error bars from the collinear laser spectroscopy result (see Table I). Combining it with the β-NMR/ON resonance frequency of 208.79(4) MHz for ^{59}Cu reported in Ref. [22], a hyperfine field value of $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.59(5)$ T is obtained. This differs by about four standard deviations from the values listed in Table I that resulted from combining resonance frequencies and magnetic moment values that were each obtained with the same experimental setups. This difference might be due to unforeseen systematic effects in this measurement [50], which was performed with a different experimental setup, as is currently being investigated [52].

C. The case of ^{67}Cu

The situation for ^{67}Cu turns out to be more complicated. In Ref. [23], the magnetic moment of ^{67}Cu obtained with the Oxford LTNO setup is given as $\mu(^{67}\mathrm{Cu}) = +2.54(2)\mu_N$; in Ref. [53] this result is quoted as $\mu = +2.536(3)\mu_N$ (this smaller error bar most probably only reflects the statistical precision). The authors do not quote a resonance frequency value, but analysis of the resonance curve shown in Ref. [23] yields a central value of $\nu_{\mathrm{res}} = 278.38(6)$ MHz. In combination with the magnetic moment value of $\mu = +2.536\mu_N$, this yields a total magnetic field of -21.60 T. Comparing this with the hyperfine field value of $-21.8(1)$ T for copper in iron that was used in Ref. [23] and neglecting the demagnetization field (as the authors of Ref. [23] also did) yields a value of $+0.20$ T for the externally applied magnetic field instead of the value of $+0.10$ T mentioned in Refs. [23,53]. The latter value is therefore most probably a typographical error.

When combining the aforementioned resonance frequency of 278.38(6) MHz with the magnetic moment value $\mu(^{67}\mathrm{Cu}) = +2.5142(6)\mu_N$ from the laser spectroscopy experiments [26], a hyperfine field value of $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.952(15)$ T is obtained for $B_{\mathrm{ext}} = 0.20(1)$ T and with $B_{\mathrm{dem}} = 0.036(8)$ T for the foils of the Oxford team (see Sec. IV A1). If the demagnetization field is neglected, $B_{\mathrm{hf}}(\mathrm{CuFe}) = -21.988(15)$ T is obtained. Both values vary from the ones obtained for the other Cu isotopes (see Table I and Fig. 2).

Concluding, there seems to be a problem with the β-NMR/ON result for ^{67}Cu that was obtained using another experimental setup than the one used for the isotopes ^{59}Cu, ^{69}Cu, and ^{71}Cu. The origin of this may, for example, be an undetected error in the frequency calibration. We therefore did not include the β-NMR/ON result for ^{67}Cu in the hyperfine field analysis presented here.

TABLE II. Overview of hyperfine magnetic fields for Cu in Fe host reported in the literature. Note that in most cases no error bar was quoted.

B_{hf}(T)	Ref.	Method
21.0	[54]	NMR
21.77	[55]	NMR
−21.27	[56]	NMR
21.79	[57]	NMR
−21.3	[42]	Spin echo
21.8(1)	[18,19]	NMR
21.3	[58]	NMR
−21.84	[59]	NMR
16.95(51)	[60]	γ-γ PAC[a]

[a] Perturbed angular correlation.

V. PREVIOUS RESULTS

Table II lists other values for the hyperfine field of Cu in Fe that are available in the literature, most of which were obtained in classical NMR experiments at room temperature and, unfortunately, with no error being quoted. As can be seen, most values are in reasonable agreement with the new value of $-21.794(10)$ T presented here. The value from the γ-γ perturbed angular correlation measurement, which is significantly deviating from all other results, is either wrong or might be related to a different lattice site for Cu impurities in Fe.

VI. COMPARISON WITH THEORETICAL VALUES

Hyperfine fields in solids can be calculated from first principles. This allows trends in those hyperfine fields to be understood as a function of the impurity element, for example, in an iron matrix [5–11], and it allows the hyperfine field to be disentangled into contributions with a different physical origin [10,11,61,62]. We calculated the hyperfine field of Cu in Fe within the framework of density functional theory [63–65], using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional [66]. For solving the scalar-relativistic Kohn-Sham equations, we employed the augmented plane waves plus local orbitals method [65,67,68] as implemented in the WIEN2K package [69] for periodic solids. In this method the wave functions are expanded into spherical harmonics inside nonoverlapping atomic spheres of radius R_{MT} and in plane waves in the remaining space of the unit cell, i.e., the interstitial region. We took $R_{\mathrm{MT}}^{\mathrm{Fe}} = R_{\mathrm{MT}}^{\mathrm{Cu}} = 2.30$ a.u. The plane-wave expansion of the wave function in the interstitial region was truncated at a large value of $K_{\max} = 8.0/R_{\mathrm{MT}}^{\min} = 3.48$ a.u.$^{-1}$, which leads to very accurate values for the calculated hyperfine fields. A dense mesh of k-points, corresponding to a

TABLE III. Calculated values for the Fermi contact field, orbital hyperfine field, dipolar hyperfine field, and atomic dipolar hyperfine field for a Cu impurity in Fe. Spin and orbital contributions to the atomic magnetic moment for Cu (μ_B) and distance between Cu and its first Fe neighbor (Å).

	B(T)		
B_F	−25.32	μ_spin	$0.115\mu_B$
B_orb	0.60	μ_orb	$0.007\mu_B$
B_dip	−0.01	$d_\text{Cu-Fe}$	2.478Å
B_dip^at	0.00		

$20 \times 20 \times 20$ mesh for a conventional bcc unit cell for Fe, was taken. Spin-orbit coupling was taken into account by a second variational step scheme [70] using a cutoff energy $E_\text{SO} = 5.0$ Ry. The substitutional Cu impurity was modeled by a 128-atom supercell, and all atoms in the supercell were allowed to adjust their positions due to the presence of the impurity. The lattice constant for the Fe matrix was taken to be the equilibrium lattice constant for the PBE functional (2.8404 Å). These settings allow for an excellent numerical convergence of the hyperfine field.

The results of the calculations are summarized in Table III. As can be seen, the distance between the Cu impurity and its first eight Fe neighbors is expanded only slightly (0.75%) compared to the Fe-Fe distance of 2.460 Å in pure Fe. The dominant contribution to the hyperfine field is the Fermi contact term, caused by s-electron spin polarization, due to the small atomic (d-electron) magnetic moment at the Cu atom. This value can be further split into a core contribution due to 1s and 2s electrons (−8.54 T), a semicore contribution by the 3s electrons (+5.80 T), and a valence contribution by 4s electrons (−22.59 T). The result for the Fermi-contact hyperfine field can be compared with the −18.2 T that was obtained 25 years ago by the Korringa-Kohn-Rostoker Green's function method [6]. The orbital hyperfine field of Cu (0.60 T) is an order of magnitude smaller than the corresponding quantity in pure Fe, consistent with the very small atomic orbital magnetic moment of Cu. All contributions to the hyperfine field, together with the Lorenz field (0.74 T), sum to a total hyperfine field of −23.99 T. Although this is about 2 T larger than the experimental value determined in this work, this deviation is state of the art and is due to inherent limitations of the chosen exchange-correlation functional.

VII. CONCLUSION

Combining resonance frequencies for the isotopes ^{59}Cu, ^{69}Cu, and ^{71}Cu obtained from β-NMR/ON measurements with the NICOLE LTNO setup at ISOLDE, with magnetic moment values obtained for these isotopes in collinear laser spectroscopy measurements at ISOLDE, the hyperfine field of Cu impurities in iron is found to be $B_\text{hf}(\text{CuFe}) = -21.794(10)$ T. This value is in agreement with, but almost an order of magnitude more precise than, the previously adopted value of −21.8(1) T and in good agreement with predictions from *ab initio* calculations. Interpreting the differences between the hyperfine field values obtained for the individual isotopes to be due to hyperfine anomalies, the hyperfine anomalies in Fe for the isotopes considered here were found to be smaller than 3×10^{-3} (90% C.L.).

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