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Deuteron and triton magnetic moments from NMR spectra of the hydrogen molecule

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We present a theory and calculations of the nuclear magnetic shielding with finite nuclear mass effects and determine the magnetic moments of deuteron and triton using the known NMR spectra of HD and HT molecules. The results $\mu_d = 0.857\,438\,234\,6(53)\mu_N$ and $\mu_t = 2.978\,962\,471(10)\mu_N$ are more accurate and in good agreement with the currently accepted values.

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When a molecule is placed in a homogeneous magnetic field $\vec{B}$, its nuclei experience the field that is shielded by the surrounding electrons $(1-\hat{\sigma})\vec{B}$. The magnitude of the shielding factor σ, typically of the order 10^{-5}, depends on the relative distance between nuclei, which means that nuclear magnetic resonance (NMR) can be used as a tool for obtaining information on the structure of complicated molecules. However, when the molecular structure can be calculated, high-precision NMR spectra can be used to determine the relative magnitude of the nuclear magnetic moments [1]. Namely, the ratio of nuclear magnetic moments is proportional to the ratio of measured frequencies that flip the nuclear spins,

$$\frac{\mu_A(1-\sigma_A)}{\mu_B(1-\sigma_B)} = \frac{f_A}{f_B}\frac{I_A}{I_B}. \tag{1}$$

The accuracy to which μ_B is known can be transferred to μ_A provided that one knows with sufficient precision the $\sigma_A - \sigma_B$ difference. Here, we report on results of the calculation of this shielding difference for HD and HT molecules. Employing these results, we determine the magnetic moment of deuteron and triton using recent high-accuracy measurements of the proton magnetic moment [2] and the ratio of spin-flip frequencies [3–6].

Magnetic shielding of the nuclear magnetic moment due to the surrounding electrons has been first considered by Ramsey in Ref. [7] with the help of the nonrelativistic Hamiltonian in the external magnetic field. His result for the isotropic shielding factor is

$$\sigma^{(0)}(R) = \frac{\alpha^2}{3}\left[\langle\phi|\sum_b \frac{1}{x_b}|\phi\rangle + \langle\phi|\sum_a \vec{x}_a\times\vec{p}_a \frac{1}{\mathcal{E}-H}\sum_b \frac{\vec{x}_b\times\vec{p}_b}{x_b^3}|\phi\rangle\right], \tag{2}$$

where α is the fine-structure constant, $\vec{x}_b$ is the position of the electron b with respect to the nucleus, $\vec{p}_b$ is its momentum, H is the molecular Hamiltonian in the Born-Oppenheimer (BO) approximation, ϕ is the electronic BO wave function, and R is the distance between nuclei. An immediate conclusion that can be drawn from this formula is that the shielding of the proton and deuteron (triton) in the HD (HT) molecule is the same. Upon averaging with the nuclear function χ, $\sigma^{(0)} = \langle\chi|\sigma^{(0)}(R)|\chi\rangle$, the difference in the shielding still vanishes, not only for the ground state but also for any excited state. Clearly, one has to go beyond the BO approximation and also include finite nuclear mass effects in the coupling to the external magnetic field. There have been several attempts to calculate the shielding difference in HD (HT), and they are all incorrect or incomplete. In 1977, Neronov and Barzakh [4] derived the formula and obtained the result of

$$\begin{aligned}\delta\sigma(\mathrm{HD}) &\equiv \sigma_d(\mathrm{HD}) - \sigma_p(\mathrm{HD}) = 15.0\times10^{-9},\\ \delta\sigma(\mathrm{HT}) &\equiv \sigma_t(\mathrm{HT}) - \sigma_p(\mathrm{HT}) = 20.4\times10^{-9},\end{aligned} \tag{3}$$

but they started with an incomplete Hamiltonian, i.e., their formula (4) does not include the nuclear spin-orbit interaction [see $g_A - 1$ terms in Eq. (4) below]. Later, the calculations by Jaszuński *et al.* [8] simulated nonadiabatic effects by an artificial charge difference. Their result of $\delta\sigma(\mathrm{HD}) = 9\times10^{-9}$, although of the correct magnitude, is not well substantiated from the physical point of view, nor is it complete. Finally, in the most recent calculations, Golubev and Shchepkin [9] used a more realistic treatment of nonadiabatic effects, but their result of $\delta\sigma(\mathrm{HD}) = 9\times10^{-9}$ was also incomplete. Undoubtedly, the coupling of electron motion to the nuclear motion is partially responsible for the difference $\delta\sigma$, but this is not the whole effect.

A derivation of the finite nuclear mass correction to the shielding closely follows that of Refs. [7,10] and starts with the Hamiltonian for electrons and nuclei, which includes coupling to the external electromagnetic field and all possible nucleus A spin-orbit interactions, i.e., ($\hbar = c = 1$),

$$\begin{aligned}H = &\sum_a \frac{\vec{\pi}_a^2}{2m} + \frac{\vec{\pi}_A^2}{2m_A} + \frac{\vec{\pi}_B^2}{2m_B} + V - \frac{e_A}{2m_A}g_A\vec{I}_A\cdot\vec{B}\\ &+\sum_b \frac{e_A e}{4\pi}\frac{\vec{I}_A}{2m_A}\cdot\frac{\vec{r}_{Ab}}{r_{Ab}^3}\times\left[g_A\frac{\vec{\pi}_b}{m} - (g_A-1)\frac{\vec{\pi}_A}{m_A}\right]\\ &+\frac{e_A e_B}{4\pi}\frac{\vec{I}_A}{2m_A}\cdot\frac{\vec{r}_{AB}}{r_{AB}^3}\times\left[g_A\frac{\vec{\pi}_B}{m_B} - (g_A-1)\frac{\vec{\pi}_A}{m_A}\right],\end{aligned} \tag{4}$$

where $\vec{\pi} = \vec{p} - e\vec{A}$, $\vec{A}$ is an external magnetic vector potential, g_A is a g-factor of the nucleus A, which is related to the magnetic moment by $\mu_A = e_A g_A I_A/(2m_A)$, and V is a Coulomb interaction between electrons and nuclei. In order to derive a formula for the shielding constant, including the finite nuclear mass corrections, we perform two unitary transformations φ,

$$\tilde{H} = e^{-i\varphi}He^{i\varphi} + \partial_t\varphi. \tag{5}$$

The first transformation places the gauge origin at the moving nucleus A. We assume that the molecule is neutral and that the magnetic field is homogeneous and there is no electric field, so

$$\varphi_1 = \sum_a e\left(x_a^i A^i + \frac{1}{2}x_a^i x_a^j A^i_{,j}\right) + e_B\left(x_B^i A^i + \frac{1}{2}x_B^i x_B^j A^i_{,j}\right), \tag{6}$$

where $\vec{A} = \vec{A}(\vec{r}_A)$, and $\vec{x}_a = \vec{r}_a - \vec{r}_A$. The transformed momenta are

$$e^{-i\varphi_1}\pi_a^j e^{i\varphi_1} = p_a^j + \frac{e_a}{2}(\vec{x}_a \times \vec{B})^j, \tag{7}$$

$$e^{-i\varphi_1}\pi_B^j e^{i\varphi_1} = p_B^j + \frac{e_B}{2}(\vec{x}_B \times \vec{B})^j, \tag{8}$$

$$e^{-i\varphi_1}\pi_A^j e^{i\varphi_1} = p_A^j + \frac{1}{2}(\vec{D} \times \vec{B})^j, \tag{9}$$

where $\vec{D} = \sum_a e\vec{x}_a + e_B\vec{x}_B$ is the electric dipole moment operator. We can now assume that the total momentum vanishes, thus $\vec{p}_A = -\vec{p}_B - \sum_a \vec{p}_a$ and the independent position variables are $\vec{x}_a$ and $\vec{x}_B$. Consider now the electronic Schrödinger equation

$$\left(\sum_a \frac{\vec{p}_a^{\,2}}{2m} + V - \mathcal{E}\right)\phi = 0, \tag{10}$$

and the next transformation φ_2 of the form

$$\varphi_2 = -\frac{m}{m_A}\sum_a \vec{x}_a \vec{p}_B, \tag{11}$$

which simplifies the nuclear kinetic energy [see Eq. (18) below]. The electron momenta are changed to

$$p_a'^i = e^{-i\varphi_2} p_a^i e^{i\varphi_2} = p_a^i - \frac{m}{m_A}p_B^i, \tag{12}$$

and the potential

$$V' - \mathcal{E} = e^{-i\varphi_2}(V - \mathcal{E})e^{i\varphi_2} \approx V - \mathcal{E} + \frac{m}{m_A}\sum_a \vec{x}_a \vec{\nabla}_B (V - \mathcal{E}), \tag{13}$$

where we omitted higher-order terms in the electron nucleus mass ratio. The new Hamiltonian $\tilde{H}$ after both transformations with $\vec{p}_{\rm el} = \sum_a \vec{p}_a$ and $\vec{x}_{\rm el} = \sum_a \vec{x}_a$ becomes

$$\begin{aligned}\tilde{H} = {} & \sum_a \frac{1}{2m}\left(\vec{p}_a + \frac{e}{2}\vec{x}_a \times \vec{B} - \frac{m}{m_A}\vec{p}_B\right)^2 + \frac{1}{2m_B}\left(\vec{p}_B + \frac{e_B}{2}\vec{x}_B \times \vec{B}\right)^2 \\ & + \frac{1}{2\,m_A}\left(\vec{p}_B + \vec{p}_{\rm el} - \frac{\vec{D} \times \vec{B}}{2}\right)^2 + V + \frac{m}{m_A}\sum_a \vec{x}_a \vec{\nabla}_B (V - \mathcal{E}) - \frac{e_A}{2m_A} g_A \vec{I}_A \cdot \vec{B} \\ & - \sum_a \frac{e_A e}{4\pi}\frac{\vec{I}_A}{2m_A} \cdot \frac{\vec{x}_a}{x_a^3} \times \left[\frac{g_A}{m}\left(\vec{p}_a + \frac{e}{2}\vec{x}_a \times \vec{B} - \frac{m}{m_A}\vec{p}_B\right) + \frac{(g_A - 1)}{m_A}\left(\vec{p}_B + \vec{p}_{\rm el} - \frac{\vec{D} \times \vec{B}}{2}\right)\right] \\ & - \frac{e_A\, e_B}{4\pi}\frac{\vec{I}_A}{2m_A} \cdot \frac{\vec{x}_B}{x_B^3} \times \left[\frac{g_A}{m_B}\left(\vec{p}_B + \frac{e_B}{2}\vec{x}_B \times \vec{B}\right) + \frac{(g_A - 1)}{m_A}\left(\vec{p}_B + \vec{p}_{\rm el} - \frac{\vec{D} \times \vec{B}}{2}\right)\right].\end{aligned} \tag{14}$$

From this Hamiltonian one derives the shielding defined by

$$H_{\rm eff} = -\frac{e_A}{2m_A} g_A \vec{I}_A (1 - \hat{\sigma}(\vec{R}))\vec{B}. \tag{15}$$

Let us consider first the nonrelativistic Hamiltonian $H_{\rm nrel} = H + H_{\rm n}$, where

$$H = \sum_a \frac{\vec{p}_a^{\,2}}{2m} + V, \tag{16}$$

with

$$V = \frac{1}{R} + \frac{1}{x_{12}} - \frac{1}{x_1} - \frac{1}{x_2} - \frac{1}{|\vec{x}_1 + \vec{R}|} - \frac{1}{|\vec{x}_2 + \vec{R}|}, \tag{17}$$

and where

$$H_{\rm n} = \frac{\vec{p}_B^{\,2}}{2m_{\rm n}} + \frac{\left(\sum_a \vec{p}_a\right)^2}{2\,m_A} + \frac{m}{m_A}\sum_a \vec{x}_a \cdot \vec{\nabla}_B (V - \mathcal{E}), \tag{18}$$

with $m_{\rm n} = m_A m_B/(m_A + m_B)$ being the nuclear reduced mass. We assume the Born-Oppenheimer approximation and include $H_{\rm n}$ perturbatively using the nonadiabatic perturbation theory (NAPT) [11]. In the zeroth order, the shielding is given by Eq. (2). The leading nonadiabatic correction to the shielding $\hat{\sigma}^{(1)}$ is linear in the electron-nuclear mass ratio, and we split it into four parts [10]: $\sigma^{(1)} = \sigma_{\rm n} + \sigma_{\rm d} + \sigma_{\rm s} + \sigma_{\rm l}$. The explicit formulas for the isotropic shielding in H_2 and isotopomers, $e_A = e_B = -e$,

with $\vec{R} = \vec{r}_{AB} = \vec{r}_A - \vec{r}_B = -\vec{x}_B$ are

$$\sigma_{\rm n} = \frac{\alpha^2}{3}\left[2\langle\phi|\sum_b \frac{1}{x_b}\frac{1}{(\mathcal{E}-H)'}\overleftrightarrow{H}_{\rm n}|\phi\rangle + \langle\phi|\sum_a \vec{x}_a\times\vec{p}_a\frac{1}{(\mathcal{E}-H)'}(\overleftrightarrow{H}_{\rm n}-\mathcal{E}_{\rm a})\frac{1}{(\mathcal{E}-H)'}\sum_b\frac{\vec{x}_b\times\vec{p}_b}{x_b^3}|\phi\rangle\right.$$
$$\left. + \langle\phi|\overleftrightarrow{H}_{\rm n}\frac{1}{(\mathcal{E}-H)'}\sum_a\vec{x}_a\times\vec{p}_a\frac{1}{(\mathcal{E}-H)'}\sum_b\frac{\vec{x}_b\times\vec{p}_b}{x_b^3}|\phi\rangle + \langle\phi|\sum_a\vec{x}_a\times\vec{p}_a\frac{1}{(\mathcal{E}-H)'}\sum_b\frac{\vec{x}_b\times\vec{p}_b}{x_b^3}\frac{1}{(\mathcal{E}-H)'}\overleftrightarrow{H}_{\rm n}|\phi\rangle\right], \tag{19}$$

$$\sigma_{\rm d} = \frac{\alpha^2}{3}\langle\phi|\frac{1}{m_B R} - \frac{1}{m_A}\frac{(g_A-1)}{g_A}\left(\sum_b\frac{\vec{x}_b}{x_b^3}+\frac{\vec{R}}{R^3}\right)(\vec{x}_{\rm el}+\vec{R})|\phi\rangle, \tag{20}$$

$$\sigma_{\rm s} = \frac{\alpha^2}{3}\langle\phi|\sum_a\vec{x}_a\times\vec{p}_a\frac{1}{(\mathcal{E}-H)'}\left\{-\frac{1}{m_{\rm n}}\frac{\vec{R}\times\vec{P}}{R^3}\right.$$
$$\left. + \frac{1}{m_A}\left(\sum_b\frac{\vec{x}_b}{x_b^3}+\frac{\vec{R}}{R^3}\right)\times\left[\vec{P}-\frac{(g_A-1)}{g_A}(\vec{P}-\vec{p}_{\rm el})\right]\right\}|\phi\rangle, \tag{21}$$

$$\sigma_{\rm l} = \frac{\alpha^2}{3}\langle\phi|\sum_b\frac{\vec{x}_b\times\vec{p}_b}{x_b^3}\frac{1}{(\mathcal{E}-H)'}$$
$$\cdot\left[\frac{1}{m_A}(\vec{x}_{\rm el}+\vec{R})\times(2\vec{P}-\vec{p}_{\rm el}) - \frac{1}{m_{\rm n}}\vec{R}\times\vec{P}\right]|\phi\rangle, \tag{22}$$

where $\vec{P} = -i\vec{\nabla}_R$, and $\langle\phi|\overleftrightarrow{\Delta}_R|\psi\rangle = -\langle\vec{\nabla}_R\phi|\vec{\nabla}_R\psi\rangle$. The result in Ref. [10] contains a mistake in $\sigma_{\rm d}$, which we correct here.

In the numerical evaluation of Eqs. (19)–(22), the ground-state wave function is represented with the explicitly correlated Gaussian functions of the form

$$\phi_{\Sigma^+} = e^{-a_{1A}r_{1A}^2 - a_{1B}r_{1B}^2 - a_{2A}r_{2A}^2 - a_{2B}r_{2B}^2 - a_{12}r_{12}^2}. \tag{23}$$

The resolvent $1/(\mathcal{E}-H)$ includes the sum of Σ^- and Π states, which are represented as

$$\phi_{\Sigma^-} = \vec{R}\cdot(\vec{r}_{1A}\times\vec{r}_{2A})\phi_{\Sigma^+}, \tag{24}$$

$$\vec{\phi}_{\Pi} = \vec{R}\times\vec{r}_{1A}\phi_{\Sigma^+}. \tag{25}$$

All of the above matrix elements are in electronic variables, so the derivatives with respect to the internuclear distance have to be obtained in advance. For this purpose we use the fact that the total angular momentum vanishes on ϕ, so

$$\vec{R}\times\vec{\nabla}_R|\phi\rangle = -\left(\sum_b\vec{x}_b\times\vec{\nabla}_b\right)|\phi\rangle, \tag{26}$$

and from the R derivative of the Schrödinger equation in the BO approximation we get

$$\vec{\nabla}_R|\phi\rangle = \frac{1}{(\mathcal{E}-H)'}\vec{\nabla}_R(V)|\phi\rangle\,. \tag{27}$$

Since we calculate only the shielding difference, all of the terms with the reduced mass, including the most difficult Δ_R, are omitted. Calculations are performed using 128 and 256

TABLE I. Shielding as a function of the internuclear distance R. Results to be multiplied by 10^{-6}. The numerical uncertainty of $\sigma^{(0)}$ is (20), while that of $\delta\sigma$ is (2) on the last digits.

R (a.u.)	$\sigma^{(0)}$	$\delta\sigma$(HD)	$\delta\sigma$(HT)
0.00	59.936 77	∞	∞
0.10	58.308 74	0.053 997	0.069 030
0.20	54.933 43	0.030 630	0.038 311
0.40	47.435 08	0.020 577	0.025 604
0.60	41.035 38	0.018 685	0.023 329
0.80	36.014 57	0.018 680	0.023 243
1.00	32.118 10	0.019 197	0.023 663
1.10	30.504 37	0.019 486	0.023 874
1.20	29.074 46	0.019 759	0.024 044
1.30	27.804 09	0.019 991	0.024 153
1.40	26.672 56	0.020 181	0.024 201
1.50	25.662 62	0.020 324	0.024 186
1.60	24.759 25	0.020 416	0.024 107
1.70	23.949 94	0.020 464	0.023 973
1.80	23.224 07	0.020 469	0.023 792
1.90	22.572 23	0.020 436	0.023 569
2.00	21.986 84	0.020 367	0.023 308
2.10	21.461 05	0.020 261	0.023 015
2.20	20.988 70	0.020 131	0.022 700
2.30	20.565 01	0.019 973	0.022 362
2.40	20.185 30	0.019 792	0.022 010
2.50	19.845 67	0.019 587	0.021 643
2.60	19.542 83	0.019 361	0.021 265
2.70	19.273 36	0.019 117	0.020 880
2.80	19.034 52	0.018 855	0.020 488
2.90	18.823 95	0.018 570	0.020 085
3.00	18.638 83	0.018 280	0.019 688
3.20	18.337 14	0.017 652	0.018 886
3.40	18.113 34	0.016 989	0.018 092
3.60	17.952 68	0.016 308	0.017 322
3.80	17.842 09	0.015 640	0.016 598
4.00	17.769 75	0.015 002	0.015 930
4.20	17.725 68	0.014 405	0.015 320
4.40	17.701 48	0.013 866	0.014 780
4.60	17.690 67	0.013 394	0.014 311
4.80	17.688 47	0.012 976	0.013 899
5.00	17.691 28	0.012 632	0.013 557
5.20	17.696 74	0.012 344	0.013 270
5.40	17.703 34	0.012 099	0.013 023
5.60	17.710 10	0.011 889	0.012 810
5.80	17.716 48	0.011 724	0.012 638
6.00	17.722 24	0.011 584	0.012 489
∞	17.750 45	0.010 753	0.011 326

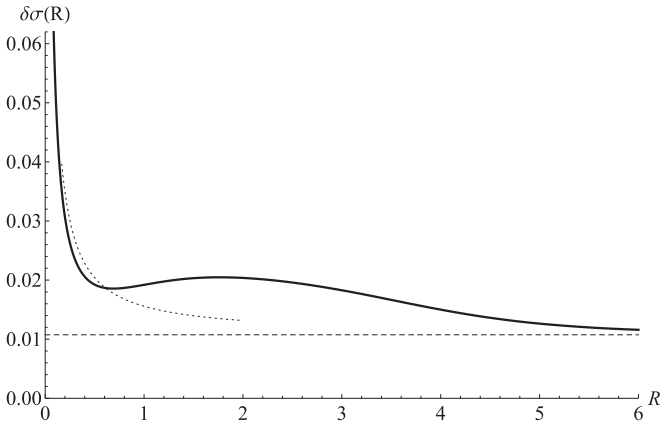

FIG. 1. The difference $\delta\sigma(\mathrm{HD},R)$ in ppm of the shielding constant between the deuteron and the proton in HD as a function of the internuclear distance R. The horizontal line is a separated atom limit, while the dotted line is the $1/R$ asymptotics that comes from the direct interaction between nuclei.

basis functions for each symmetry with global optimization of all nonlinear parameters. The numerical results in the range $R \in \langle 0,6\rangle$ a.u. are presented in Table I. Although the results for $R > 3$ are not in principle needed, we use them for testing against the known separated atom limit, which is

$$\lim_{R\to\infty} \sigma^{(1)}(R) = -\frac{\alpha^2}{3}\frac{m}{M}\left(1+\frac{g_A-1}{g_A}\right). \tag{28}$$

On the other hand, at small R we observe $1/R$ behavior, which is not an artifact but a result of the shielding of the nucleus A by the nucleus B (see Fig. 1). Our results at $R = 1.4$ a.u. in comparison to the known previous calculations are presented in Table II.

The total isotropic magnetic shielding σ is obtained by averaging with the nuclear wave function $\chi, \sigma = \langle\chi|\sigma^{(0)}(R) + \sigma^{(1)}(R)|\chi\rangle$, where χ is a solution of the nuclear radial equation with the BO potential augmented by adiabatic correction. Since the measurement [3] was performed at $T = 300$ K, we include contributions from the excited rotational states up to $J = 9$, according to the Boltzmann distribution. The averaged result for the (Ramsey) shielding factor of the H_2 and isotopomers is $\sigma^{(0)} = 26.335\,17(20) \times 10^{-6}$. However, $\sigma^{(0)}$ does not include relativistic corrections that are of the relative order of $\alpha^2 \sim 10^{-4}$. The related estimate from Ref. [8] is much

TABLE II. Extrapolation to a complete basis and comparison with the previous calculations of the isotropic nonrelativistic BO shielding in HD (HT) at $R = 1.4$ a.u. Results to be multiplied by 10^{-6}.

Size/Ref.	$\sigma_{\mathrm{el}}^{(0)}$	$\delta\sigma$(HD)	$\delta\sigma$(HT)
128	26.673 193	0.020 188 2	0.024 214 5
256	26.672 556	0.020 181 2	0.024 201 0
512	26.672 422	0.020 179 9	0.024 199 6
∞	26.672 387(35)	0.020 179 6(3)	0.024 199 4(2)
[12] (1995)	26.813 9		
[13] (1996)	26.680		
[8] (2011)	26.677 111		

TABLE III. Determination of the deuteron and the triton magnetic moments. μ_p(HD) denotes the shielded magnetic moment of the proton in HD molecules. The relative uncertainty 10^{-3} of $\delta\sigma$ comes from the neglected higher-order m/m_{n} corrections and relativistic effects are expected to be ten times smaller.

	Value	Ref.
μ_p	2.792 847 350(9) μ_N	[2]
$\delta\sigma(\mathrm{HD}, T = 300\ \mathrm{K})$	$0.020\,20(2) \times 10^{-6}$	This work
$\mu_p(\mathrm{HD})/\mu_d(\mathrm{HD})$	3.257 199 514(21)	[3]
	3.257 199 531(29)	[5]
	3.257 199 520(17)	Averaged
$\mu_d = \mu_d(\mathrm{HD})/\mu_p(\mathrm{HD})$	0.857 438 234 6(53)μ_N	This work
$\times(1+\delta\sigma)\mu_p$	0.857 438 230 8(72)μ_N	[14]
$\delta\sigma(\mathrm{HT}, T = 300\ \mathrm{K})$	$0.024\,14(2) \times 10^{-6}$	This work
$\mu_t(\mathrm{HT})/\mu_p(\mathrm{HT})$	1.066 639 893 3(7)	[6]
$\mu_t = \mu_t(\mathrm{HT})/\mu_p(\mathrm{HT})$	2.978 962 471(10)μ_N	This work
$\times(1+\delta\sigma)$	2.978 962 448(38)μ_N	[14]

smaller than the relativistic correction to the shielding of the individual hydrogen atoms, so it is possibly incorrect. The shielding differences in HD and HT are presented in Table III. Their uncertainties come from the unknown higher-order nonadiabatic corrections. From these differences and from Eq. (1) we obtain the magnetic moments of deuteron and triton (see Table III). The ratio of shielded magnetic moments for HD is the average of two independent and consistent measurements [3–5]. The obtained result for μ_d is more accurate and in good agreement with the presently accepted value, which was obtained from an unpublished experimental result by Philips *et al.* (1984) (see Ref. [14] for details). Regarding μ_t, the Committee on Data for Science and Technology (CODATA) [14] value is based on the earlier, less accurate work [5], while we use a more recent one [6] and correct the value for $\delta\sigma$, which leads to an even smaller uncertainty of μ_t. We should note, however, that the result of Ref. [6] needs confirmation as the pressure dependence has not been studied there, and because of the lack of information on the temperature, which we assumed to be $T = 300$ K.

In summary, we have determined improved values for the deuteron and triton magnetic moments. This demonstrates that NMR spectroscopy, combined with precise calculations of the shielding factor, may lead to a very accurate determination of nuclear magnetic moments. Moreover, one may consider improving the determination of magnetic moments of other light nuclei, such as ^{3}He, since the shielding factor for molecular hydrogen can be calculated including nonadiabatic and relativistic effects, as has been already done for the ^{3}He atom [15].

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