

## Supplementary Part

**Table S1.** Preferred values of magnetic moments of light nuclei shown in different units.

Nucleus (spin)	$\mu_X/\mu_N$	Reference	$\mu_X/\mu_N^{\text{length}}$	g <sub>X</sub> factor/ $\mu_N$	$\gamma_X \times 10^7 \text{ rad s}^{-1} \text{ T}^{-1}$
<sup>1</sup> H(1/2)	2.79284734463(82)	[2]	4.8373534775(14)	5.58569468924(164)	26.75221894(8)
<sup>2</sup> H(1)	0.8574382346(53)	[2,33]	1.714876318(11)	0.8574382346(53)	4.10662893(2)
<sup>3</sup> H(1/2)	2.978962471(10)	[2,34]	5.159714331(17)	5.957924942(20)	28.5349847(1)
<sup>3</sup> He(1/2)	2.127625308(25)	[68]	3.685155117(43)	4.255250616(50)	20.3801695(2)
<sup>6</sup> Li(1)	0.8220454(25)	[54]	1.1625481(71)	0.8220457(50)	3.937119(2)
<sup>7</sup> Li(3/2)	3.2564171(98)	[54]	4.2040170(26)	2.17094533(13)	10.3975616(6)
<sup>9</sup> Be(3/2)	1.17743159(3)	[59]	1.52005759(4)	0.78495439(2)	3.759474(2)
<sup>10</sup> B(3)	1.8004636(8)	[52]	2.0789962(9)	0.6001545(3)	2.874390(1)
<sup>11</sup> B(3/2)	2.6883781(11)	[52]	3.4706811(14)	1.7922521(7)	8.583842(3)

### 1. Materials and Methods

The experimental conditions of many results collected in our lab one can find in the original papers [18,19,42,43,50,52,53,68]. Completely new results were achieved in the conditions described in detail below. All spectra were measured using Varian-INOVA 500 ( $B_0=11.744 \text{ T}$ ) spectrometer at a constant temperature of 300K.

#### 1.1. Deuterium measurements.

Nine ampoules 4mm o.d. and 0.35 mL of volume with HD (Isotec, 98%D) in the pressure range 3 – 23 atm were prepared in a glass vacuum apparatus using liquid helium as a refrigerator. These samples were kept in the standard 5mm NMR tubes with nitromethane- $d_3$  as the lock substance. The <sup>1</sup>H and <sup>2</sup>H(D) NMR spectra were measured at 500.6 and 76.8464 MHz. Deuterium spectra were accumulated by INEPT optimized by spin-spin coupling <sup>1</sup>J(<sup>2</sup>H/<sup>1</sup>H)~43 Hz sequence and without a lock stabilization system. The lock drift of the superconducting magnet was previously checked as 4Hz over 24 hours. The mean acquisition time of each experiment was no longer than a few minutes.

#### 1.2. <sup>7</sup>Li experiments

CH<sub>3</sub>COOLi and LiBF<sub>4</sub>, studied in water solutions, were obtained from Sigma-Aldrich: CH<sub>3</sub>COOLi (lithium acetate dehydrate, 98%), LiBF<sub>4</sub> (lithium tetrafluoroborate, 98%). 10 samples of each salt were prepared by dissolving in distilled water, freezing in a 4mm outer diameter glass tube and blowing by torch under vacuum after degassing. Naturally abundance <sup>6</sup>Li, <sup>11</sup>B, <sup>13</sup>C and <sup>19</sup>F NMR spectra was measured and appropriate parameters was noted. All measurements were performed in the usual analytical conditions on Varian sw5 probe. Bulk susceptibility corrections were made for neat water  $\sigma(300\text{K})=-3.005 \text{ ppm}$  for the infinite dilution solution according to  $\chi_M=-18.9(\text{cgs})$ ,  $M_m=18.09$  and  $\rho(300\text{K})=1.0006 \text{ (g/cm}^3\text{)}$ . Unfortunately, the absolute shielding constant of <sup>6</sup>Li NMR reference, 9.7M LiCl in D<sub>2</sub>O solution, is not known. As a consequence, the  $\sigma_0(^{6/7}\text{Li})$  in Table 5 cannot be exactly accomplished.

#### 1.3. Beryllium investigations

In our new reinvestigation project, we have taken the BeSO<sub>4</sub> water solutions with helium-3 as additional reference component. In order to verify the conformity of the nuclear shielding values of beryllium nuclei in water solutions we have utilize Equation 1 with <sup>3</sup>He frequency and the best known value the nuclear magnetic dipole moment of  $\mu(^9\text{Be})=-1.17743159(3)\mu_N$  [59]. We found a new shielding value of

beryllium cations in water with solvent effect  $\sigma(^9\text{Be}^{+2}) = 110.16(5)$  ppm, slightly lower than that of last theoretical results [57].

$\text{BeSO}_4 \times 4\text{H}_2\text{O}$  (99%, Sigma-Aldrich) was used without further purification. Nine solutions of concentrations from 0.005 up to 0.68 mol/L were prepared in 4 mm o.d. Pyrex glass tubes (approx. 5.5 cm long). Liquid samples were degassed by several recurrent freeze-thaw pump cycles and then sealed. The pH exponent of all solutions prepared was checked as equal 3-4. The low concentrations and acidity of solutions preserve the formation of polynuclear complexes of beryllium cations. Small amounts of helium-3 were included before melting the glass samples. The samples were then fitted into standard 5 mm o.d. thin-walled NMR tubes (Wilmad 528-PP) with liquid  $\text{D}_2\text{O}$  in the annular space. The deuterium signal in the external heavy water was used for the lock system and as the primary reference standard. The constant frequency of the lock system (76.8464 MHz) made it possible to preserve the same  $B_0$  for all measurements. The  $^1\text{H}$ ,  $^3\text{He}$  and  $^9\text{Be}$  NMR spectra were recorded on a Varian UNITY-Plus 500 FT spectrometer operating at 500.6074, 381.8777 and 178.3775 MHz, respectively. For  $^1\text{H}$  spectra, liquid TMS, and for beryllium nuclei, 0.43M solution of  $\text{Be}^{+2}$  in  $\text{D}_2\text{O}$ , were taken as external standards.

#### 1.4. $^3\text{He}$ , $^{10}\text{B}$ and $^{11}\text{B}$ spectra

Experimental data of our  $^{10}\text{B}$  and  $^{11}\text{B}$  measurements performed in the gas phase were presented in [52] in details. Here the appropriate NMR spectra recorded at different densities are shown.