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ANNOUNCEMENT

NMR Nomenclature: Nuclear Spin Properties and Conventions for Chemical Shifts—IUPAC Recommendations

Scientific advances are facilitated by the international adoption of standardised notation and by the establishment of accurate numerical values for many physical quantities. The body charged with oversight of these areas for chemists is the International Union of Pure and Applied Chemistry (IUPAC). Its first attempts at standardisation of NMR data appeared (*1, 2*) in the 1970s. These publications established the conventions for chemical shifts and generally have stood the test of time. The famous "Green Book" titled *Quantities, Units and Symbols in Physical Chemistry* (*3*) contains, *inter alia*, a table of the properties of all the known nuclides. Recently, the IUPAC has turned its attention again to NMR and has issued six new sets of recommendations, (*4–9*), all published in the IUPAC journal *Pure and Applied Chemistry*. Three of these (*4–6*) deal with computerized databases and representation of pulse sequences. One recommends (*7*) NMR parameters and symbols to be used in publications.

Reference (*8*), which is described here, updates the recommendations with regard to chemical shifts. It discusses the methods of referencing spectra and recommends that shifts of *all*

TABLE 1
The Spin Properties of Spin-1/2 Nuclei

Isotope	Natural abundance (x/%)	Magnetic moment (μ/μ_N)	Magnetogyric ratio ($\gamma/10^7$rad s^{-1} T^{-1})	Frequency ratio (Ξ/%)	Reference compound	Sample conditions	Relative receptivity	
							D^P	D^C
^{1}H	99.9885	4.837 353 570	26.752 2128	100.000 000	Me_4Si	$CDCl_3$, $\varphi = 1\%$	1.000	5.87×10^{3}
^{3}H	—	5.159 714 367	28.534 9779	106.663 974	Me_4Si-t_1	See lit.	—	—
^{3}He	1.37×10^{-4}	−3.685 154 336	−20.380 1587	76.179 437	He	Gas	6.06×10^{-7}	3.56×10^{-3}
^{13}C	1.07	1.216 613	6.728 284	25.145 020	Me_4Si	$CDCl_3$, $\varphi = 1\%$	1.70×10^{-4}	1.00
^{15}N	0.368	−0.490 497 46	−2.712 618 04	10.136 767	$MeNO_2$	Neat/$CDCl_3$	3.84×10^{-6}	2.25×10^{-2}
^{19}F	100	4.553 333	25.181 48	94.094 011	CCl_3F	See lit.	0.834	4.90×10^{3}
^{29}Si	4.6832	−0.961 79	−5.3190	19.867 187	Me_4Si	$CDCl_3$, $\varphi = 1\%$	3.68×10^{-4}	2.16
^{31}P	100	1.959 99	10.8394	40.480 742	H_3PO_4	See lit.	6.65×10^{-2}	3.91×10^{2}
^{57}Fe	2.119	0.156 9636	0.868 0624	3.237 778	$Fe(CO)_5$	C_6D_6	7.24×10^{-7}	4.25×10^{-3}
^{77}Se	7.63	0.926 775 77	5.125 3857	19.071 513	Me_2Se	Neat/C_6D_6	5.37×10^{-4}	3.15
^{89}Y	100	−0.238 010 49	−1.316 2791	4.900 198	$Y(NO_3)_3$	H_2O/D_2O	1.19×10^{-4}	0.700
^{103}Rh	100	−0.1531	−0.8468	3.186 447	$Rh(acac)_3$	$CDCl_3$, sat.	3.17×10^{-5}	0.186
(^{107}Ag)	51.839	−0.196 898 93	−1.088 9181	4.047 819	$AgNO_3$	D_2O, sat.	3.50×10^{-5}	0.205
^{109}Ag	48.161	−0.226 362 79	−1.251 8634	4.653 533	$AgNO_3$	D_2O, sat.	4.94×10^{-5}	0.290
(^{111}Cd)	12.80	−1.030 3729	−5.698 3131	21.215 480	Me_2Cd	Neat	1.24×10^{-3}	7.27
^{113}Cd	12.22	−1.077 8568	−5.960 9155	22.193 175	Me_2Cd	Neat	1.35×10^{-3}	7.94
(^{115}Sn)	0.34	−1.5915	−8.8013	32.718 749	Me_4Sn	Neat/C_6D_6	1.21×10^{-4}	0.711
(^{117}Sn)	7.68	−1.733 85	−9.588 79	35.632 259	Me_4Sn	Neat/C_6D_6	3.54×10^{-3}	20.8
^{119}Sn	8.59	−1.813 94	−10.0317	37.290 632	Me_4Sn	Neat/C_6D_6	4.53×10^{-3}	26.6
(^{123}Te)	0.89	−1.276 431	−7.059 098	26.169 742	Me_2Te	Neat/C_6D_6	1.64×10^{-4}	0.961
^{125}Te	7.07	−1.538 9360	−8.510 8404	31.549 769	Me_2Te	Neat/C_6D_6	2.28×10^{-3}	13.4
^{129}Xe	26.44	−1.347 494	−7.452 103	27.810 186	$XeOF_4$	Neat	5.72×10^{-3}	33.6
^{183}W	14.31	0.204 009 19	1.128 2403	4.166 387	Na_2WO_4	D_2O, 1 M	1.07×10^{-5}	6.31×10^{-2}
^{187}Os	1.96	0.111 9804	0.619 2895	2.282 331	OsO_4	CCl_4, 0.98 M	2.43×10^{-7}	1.43×10^{-3}
^{195}Pt	33.832	1.0557	5.8385	21.496 784	Na_2PtCl_6	D_2O, 1.2 M	3.51×10^{-3}	20.7
^{199}Hg	16.87	0.876 219 37	4.845 7916	17.910 822	Me_2Hg^a	Neat	1.00×10^{-3}	5.89
(^{203}T1)	29.524	2.809 833 05	15.539 3338	57.123 200	$T1(NO_3)_3$	See lit.	5.79×10^{-2}	3.40×10^{2}
^{205}T1	70.476	2.837 470 94	15.692 1808	57.683 838	$T1(NO_3)_3$	See lit.	0.142	8.36×10^{2}
^{207}Pb	22.1	1.009 06	5.580 46	20.920 599	Me_4Pb	Neat/C_6D_6	2.01×10^{-3}	11.8

Note. Taken from *Pure Appl. Chem.* **73,** 1795 (2001). © IUPAC 2001 Full text at http://www.iupac.org/publications/pac/2001/7311/7311x1795.html.
[a] Highly toxic. Do not handle directly. Some other reference compounds are toxic. The unified scale should always be used in these cases.

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TABLE 2
The Spin Properties of Quadrupolar Nuclei

Isotope	Spin	Natural abundance (x/%)	Magnetic moment (μ/μ_N)	Magnetogyric ratio ($\gamma/10^7$rad s^{-1} T^{-1})	Quadrupole moment (Q/fm^2)	Frequency ratio (Ξ/%)	Reference sample	Sample conditions	Line-width factor(ℓ/fm^4)	Relative receptivity	
										D^p	D^C
^{2}H	1	0.0115	1.212 600 77	4.106 627 91	0.2860	15.350 609	$(CD_3)_4Si$	$CDCl_3$ $\varphi = 1\%$	0.41	1.11×10^{-6}	6.52×10^{-3}
^{6}Li	1	7.59	1.162 5637	3.937 1709	−0.0808	14.716 086	LiCl	D_2O, 9.7 m	0.033	6.45×10^{-4}	3.79
^{7}Li	3/2	92.41	4.204 075 05	10.397 7013	−4.01	38.863 797	LiCl	D_2O, 9.7 m	21	0.271	1.59×10^{3}
^{9}Be	3/2	100	−1.520 136	−3.759 666	5.288	14.051 813	$BeSO_4$	D_2O, 0.43 m	37	1.39×10^{-2}	81.5
^{10}B	3	19.9	2.079 2055	2.874 6786	8.459	10.743 658	$BF_3{\cdot}Et_2O$	$CDCl_3$	14	3.95×10^{-3}	23.2
^{11}B	3/2	80.1	3.471 0308	8.584 7044	4.059	32.083 974	$BF_3{\cdot}Et_2O$	$CDCl_3$	22	0.132	7.77×10^{2}
^{14}N	1	99.632	0.571 004 28	1.933 7792	2.044	7.226 317	CH_3NO_2	Neat/$CDCl_3$	21	1.00×10^{-3}	5.90
^{17}O	5/2	0.038	−2.240 77	−3.628 08	−2.558	13.556 457	D_2O	Neat	2.1	1.11×10^{-5}	6.50×10^{-2}
^{21}Ne	3/2	0.27	−0.854 376	−2.113 08	10.155	7.894 296	Ne	Gas, 1.1 MPa	140	6.65×10^{-6}	3.91×10^{-2}
^{23}Na	3/2	100	2.862 9811	7.080 8493	10.4	26.451 900	NaCl	D_2O, 0.1 M	140	9.27×10^{-2}	5.45×10^{2}
^{25}Mg	5/2	10.00	−1.012 20	−1.638 87	19.94	6.121 635	$MgCl_2$	D_2O, 11 M	130	2.68×10^{-4}	1.58
^{27}Al	5/2	100	4.308 6865	6.976 2715	14.66	26.056 859	$Al(NO_3)_3$	D_2O, 1.1 m	69	0.207	1.22×10^{3}
^{33}S	3/2	0.76	0.831 1696	2.055 685	−6.78	7.676 000	$(NH_4)_2SO_4$	D_2O, sat.	61	1.72×10^{-5}	0.101
^{35}Cl	3/2	75.78	1.061 035	2.624 198	−8.165	9.797 909	NaCl	D_2O, 0.1 M	89	3.58×10^{-3}	21.0
^{37}Cl	3/2	24.22	0.883 1998	2.184 368	−6.435	8.155 725	NaCl	D_2O, 0.1 M	55	6.59×10^{-4}	3.87
^{39}K	3/2	93.2581	0.505 433 76	1.250 0608	5.85	4.666 373	KCl	D_2O, 0.1 M	46	4.76×10^{-4}	2.79
(^{40}K)	4	0.0117	−1.451 3203	−1.554 2854	−7.3	5.802 018	KCl	D_2O, 0.1 M	5.2	6.12×10^{-7}	3.59×10^{-3}
(^{41}K)	3/2	6.7302	0.277 396 09	0.686 068 08	7.11	2.561 305	KCl	D_2O, 0.1 M	67	5.68×10^{-6}	3.33×10^{-2}
^{43}Ca	7/2	0.135	−1.494 067	−1.803 069	−4.08	6.730 029	$CaCl_2$	D_2O, 0.1 M	2.3	8.68×10^{-6}	5.10×10^{-2}
^{45}Sc	7/2	100	5.393 3489	6.508 7973	−22.0	24.291 747	$Sc(NO_3)_3$	D_2O, 0.06 M	66	0.302	1.78×10^{3}
^{47}Ti	5/2	7.44	−0.932 94	−1.5105	30.2	5.637 534	$TiCl_4$	Neat	290	1.56×10^{-4}	0.918
^{49}Ti	7/2	5.41	−1.252 01	−1.510 95	24.7	5.639 037	$TiCl_4$	Neat	83	2.05×10^{-4}	1.20
(^{50}V)	6	0.250	3.613 7570	2.670 6490	21.0	9.970 309	$VOCl_3$	Neat/C_6D_6	17	1.39×10^{-4}	0.818
^{51}V	7/2	99.750	5.838 0835	7.045 5117	−5.2	26.302 948	$VOCl_3$	Neat/C_6D_6	3.7	0.383	2.25×10^{3}
^{53}Cr	3/2	9.501	−0.612 63	−1.5152	−15.0	5.652 496	K_2CrO_4	D_2O, sat.	300	8.63×10^{-5}	0.507
^{55}Mn	5/2	100	4.104 2437	6.645 2546	33.0	24.789 218	$KMnO_4$	D_2O, 0.82 m	350	0.179	1.05×10^{3}
^{59}Co	7/2	100	5.247	6.332	42.0	23.727 074	$K_3[Co(CN)_6]$	D_2O, 0.56 m	240	0.278	1.64×10^{3}
^{61}Ni	3/2	1.1399	−0.968 27	−2.3948	16.2	8.936 051	$Ni(CO)_4$	Neat/C_6D_6	350	4.09×10^{-5}	0.240
^{63}Cu	3/2	69.17	2.875 4908	7.111 7890	−22.0	26.515 473	$[Cu(CH_3CN)_4][ClO_4]$	CH_3CN, sat.	650	6.50×10^{-2}	3.82×10^{2}
^{65}Cu	3/2	30.83	3.074 65	7.604 35	−20.4	28.403 693	$[Cu(CH_3CN)_4][ClO_4]$	CH_3CN, sat.	550	3.54×10^{-2}	2.08×10^{2}
^{67}Zn	5/2	4.10	1.035 556	1.676 688	15.0	6.256 803	$Zn(NO_3)_2$	D_2O, sat.	72	1.18×10^{-4}	0.692
(^{69}Ga)	3/2	60.108	2.603 405	6.438 855	17.1	24.001 354	$Ga(NO_3)_3$	D_2O, 1.1 m	390	4.19×10^{-2}	2.46×10^{2}
^{71}Ga	3/2	39.892	3.307 871	8.181 171	10.7	30.496 704	$Ga(NO_3)_3$	D_2O, 1.1 m	150	5.71×10^{-2}	3.35×10^{2}
^{73}Ge	9/2	7.73	−0.972 2881	−0.936 0303	−19.6	3.488 315	$(CH_3)_4Ge$	Neat	28	1.09×10^{-4}	0.642
^{75}As	3/2	100	1.858 354	4.596 163	31.4	17.122 614	$NaAsF_6$	CD_3CN, 0.5 M	1300	2.54×10^{-2}	1.49×10^{2}

(^{79}Br)	3/2	50.69	2.719 351	6.725 616	31.3	25.053 980	NaBr	D_2O, 0.01 M	1300	4.03×10^{-2}	2.37×10^{2}
^{81}Br	3/2	49.31	2.931 283	7.249 776	26.2	27.006 518	NaBr	D_2O, 0.01 M	920	4.91×10^{-2}	2.88×10^{2}
^{83}Kr	9/2	11.49	−1.073 11	−1.033 10	25.9	3.847 600	Kr	Gas	50	2.18×10^{-4}	1.28
(^{85}Rb)	5/2	72.17	1.601 3071	2.592 7050	27.6	9.654 943	RbCl	D_2O, 0.01 M	240	7.67×10^{-3}	45.0
^{87}Rb	3/2	27.83	3.552 582	8.786 400	13.35	32.720 454	RbCl	D_2O, 0.01 M	240	4.93×10^{-2}	2.90×10^{2}
^{87}Sr	9/2	7.00	−1.209 0236	−1.163 9376	33.5	4.333 822	$SrCl_2$	D_2O, 0.5 M	83	1.90×10^{-4}	1.12
^{91}Zr	5/2	11.22	−1.542 46	−2.497 43	−17.6	9.296 298	$Zr(C_5H_5)_2Cl_2$	CH_2Cl_2, sat.	99	1.07×10^{-3}	6.26
^{93}Nb	9/2	100	6.8217	6.5674	−32.0	24.476 170	$K[NbCl_6]$	CH_3CN, sat.	76	0.488	2.87×10^{3}
^{95}Mo	5/2	15.92	−1.082	−1.751	−2.2	6.516 926	Na_2MoO_4	D_2O, 2 M	1.5	5.21×10^{-4}	3.06
(^{97}Mo)	5/2	9.55	−1.105	−1.788	25.5	6.653 695	Na_2MoO_4	D_2O, 2 M	210	3.33×10^{-4}	1.95
^{99}Tc	9/2	—	6.281	6.046	−12.9	22.508 326	NH_4TcO_4	D_2O	12	—	—
^{99}Ru	5/2	12.76	−0.7588	−1.229	7.9	4.605 151	$K_4[Ru(CN)_6]$	D_2O, 0.3 M	20	1.44×10^{-4}	0.848
^{101}Ru	5/2	17.06	−0.8505	−1.377	45.7	5.161 369	$K_4[Ru(CN)_6]$	D_2O, 0.3 M	670	2.71×10^{-4}	1.59
^{105}Pd	5/2	22.33	−0.760	−1.23	66.0	4.576 100	K_2PdCl_6	D_2O, sat.	1400	2.53×10^{-4}	1.49
(^{113}In)	9/2	4.29	6.1124	5.8845	79.9	21.865 755	$In(NO_3)_3$	D_2O, 0.1 M	470	1.51×10^{-2}	88.5
^{115}In	9/2	95.71	6.1256	5.8972	81.0	21.912 629	$In(NO_3)_3$	D_2O, 0.1 M	490	0.338	1.98×10^{3}
^{121}Sb	5/2	57.21	3.9796	6.4435	−36.0	23.930 577	$KSbCl_6$	CH_3CN, sat.	410	9.33×10^{-2}	5.48×10^{2}
(^{123}Sb)	7/2	42.79	2.8912	3.4892	−49.0	12.959 217	$KSbCl_6$	CH_3CN, sat.	330	1.99×10^{-2}	1.17×10^{2}
^{127}I	5/2	100	3.328 710	5.389 573	−71.0	20.007 486	KI	D_2O, 0.01 M	1600	9.54×10^{-2}	5.60×10^{2}
^{131}Xe	3/2	21.18	0.893 1899	2.209 076	−11.4	8.243 921	$XeOF_4$	Neat	170	5.96×10^{-4}	3.50
^{133}Cs	7/2	100	2.927 7407	3.533 2539	−0.343	13.116 142	$CsNO_3$	D_2O, 0.1 M	0.016	4.84×10^{-2}	2.84×10^{2}
(^{135}Ba)	3/2	6.592	1.081 78	2.675 50	16.0	9.934 457	$BaCl_2$	D_2O, 0.5 M	340	3.30×10^{-4}	1.93
^{137}Ba	3/2	11.232	1.210 13	2.992 95	24.5	11.112 928	$BaCl_2$	D_2O, 0.5 M	800	7.87×10^{-4}	4.62
^{138}La	5	0.090	4.068 095	3.557 239	45.0	13.194 300	$LaCl_3$	D_2O/H_2O	120	8.46×10^{-5}	0.497
^{139}La	7/2	99.910	3.155 6770	3.808 3318	20.0	14.125 641	$LaCl_3$	D_2O, 0.01 M	54	6.05×10^{-2}	3.56×10^{2}
^{177}Hf	7/2	18.60	0.8997	1.086	336.5	(4.007)	—	—	1.5×10^{4}	2.61×10^{-4}	1.54
^{179}Hf	9/2	13.62	−0.7085	−0.6821	379.3	(2.517)	—	—	1.1×10^{4}	7.45×10^{-5}	0.438
^{181}Ta	7/2	99.988	2.6879	3.2438	317.0	11.989 600	$KTaCl_6$	CH_3CN, sat.	1.4×10^{4}	3.74×10^{-2}	2.20×10^{2}
(^{185}Re)	5/2	37.40	3.7710	6.1057	218.0	22.524 600	$KReO_4$	D_2O, 0.1 M	1.5×10^{4}	5.19×10^{-2}	3.05×10^{2}
^{187}Re	5/2	62.60	3.8096	6.1682	207.0	22.751 600	$KReO_4$	D_2O, 0.1 M	1.4×10^{4}	8.95×10^{-2}	5.26×10^{2}
^{189}Os	3/2	16.15	0.851 970	2.107 13	85.6	7.765 400	OsO_4	CCl_4, 0.98 M	9800	3.95×10^{-4}	2.32
(^{191}Ir)	3/2	37.3	0.1946	0.4812	81.6	(1.718)	—	—	8900	1.09×10^{-5}	6.38×10^{-2}
^{193}Ir	3/2	62.7	0.2113	0.5227	75.1	(1.871)	—	—	7500	2.34×10^{-5}	0.137
^{197}Au	3/2	100	0.191 271	0.473 060	54.7	(1.729)	—	—	4000	2.77×10^{-5}	0.162
^{201}Hg	3/2	13.18	−0.723 2483	−1.788 769	38.6	6.611 583	$(CH_3)_2Hg$[a]	Neat	2000	1.97×10^{-4}	1.16
^{209}Bi	9/2	100	4.5444	4.3750	−51.6	16.069 288	$Bi(NO_3)_2$	$HNO_3/D_2O/H_2O$	200	0.144	8.48×10^{2}

Note. Taken from *Pure Appl. Chem.* **73,** 1795 (2001). © IUPAC 2001. Full text at http://www.iupac.org/publications/pac/7311/7311x1795.html.

[a] Highly toxic. Do not handle directly. Some other reference compounds are toxic. The unified scale should always be used in these cases.

nuclides be reported on a unified scale relative to the primary standard, which is the proton resonance of tetramethylsilane in dilute solution (volume fraction $\phi < 1\%$) in chloroform. Such a scale is given the symbol Ξ (capital Greek xi) and is expressed as a ratio (generally in %) of the resonance frequency in question to that of the primary standard. However, it is recognised that it will remain common to relate shifts to standards specific to each nucleus, so to facilitate conversion to the Ξ scale, standard substances are proposed and their values of Ξ quoted for all nonradioactive NMR-active nuclides (excluding lanthanides and actinides). Tables 1 and 2 summarise such information in a simplified way (without the literature references and footnotes). However, before making use of the data on Ξ, readers should check with the additional information in the full tables in Ref. (*8*). Many earlier IUPAC recommendations on NMR are endorsed, but the δ-scale for nuclide-specific shifts is redefined so that the fractional "dimension" (e.g., ppm) must be specifically reported. Nine new recommendations relating to chemical shifts are made. Moreover, significant nuclear spin data, such as isotopic abundances, magnetogyric ratios, and quadrupole moments, are given in tabular form, updated from Ref. (*3*).

The use of a unified scale for reporting chemical shifts of five nuclides commonly studied in proteins and nucleic acids in aqueous solution has previously been the subject of a joint IUPAC/IUBMB/IUPAB recommendion (*9*) which is now in common use. In that case the recommended primary reference is the proton resonance of DSS [sodium 2,2-dimethyl-2-silapentane-5-sulfonate, $Me_3SiCD_2CD_2CD_2SO_3Na$, which is more properly called sodium 3-(trimethylsilyl)propane-1-sulfonate]. However, the TMS and DSS scales have been shown to be virtually identical (*8, 9*).

IUPAC is keen to see its recommendations widely publicised, and it therefore publishes these freely on the Web. Thus, Ref. (*8*) can be accessed at http://www.iupac.org/publications/pac/2001/7311/7311x1795.html. The information can be copied and reproduced subject only to (a) proper acknowledgment of the original *Pure Appl. Chem.* article, and (b) retention of the copyright with IUPAC.

NMR spectroscopists are urged to read the document (*8*) and to adhere to its recommendations.

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