NUCLEAR SPINS, MOMENTS, AND OTHER DATA RELATED TO NMR SPECTROSCOPY

This table presents the following data relevant to nuclear magnetic resonance spectroscopy:

Z: Atomic number

Isotope: Element symbol and mass number

Abundance: Natural abundance of the isotope in percent. An * indicates a radioactive nuclide; if no value is given, the nuclide is not present in nature or its abundance is highly variable.

I: Nuclear spin

v: Resonant frequency in megahertz for an applied field H_0 of 1 tesla (in cgs units, 10 kilogauss). The resonant frequency scales with H_0.

Relative sensitivity: Sensitivity relative to ^{1}H (=1) assuming an equal number of nuclei and constant temperature. Values were calculated from the expressions:

For constant H_0: $0.0076508(\mu/\mu_N)^3(I + 1)/I^2$
For constant ν: $0.23871(\mu/\mu_N)(I + 1)$

μ/μ_N: Nuclear magnetic moment in units of the nuclear magneton μ_N

Q: Nuclear quadrupole moment in units of femtometers squared (1 fm^2 = 10^{-2} barn). Because the determination of quadrupole moments requires knowledge of the electron configuration near the nucleus, values of *Q* in the literature tend to scatter considerably. The values quoted here come mainly from the review of Pyykkö (Ref. 3), otherwise from Ref. 1.

The table includes all stable nuclides of non-zero spin for which spin and magnetic moment values have been measured, as well as selected radioactive nuclides of current or potential interest. At least one isotope is included for each element through *Z* = 95 for which data are available. See Reference 1 for a complete listing of spins and moments.

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References

1. Holden, N. E., "Table of the Isotopes", in Lide, D. R., Ed., *CRC Handbook of Chemistry and Physics*, 90th Ed., CRC Press, Boca Raton, FL, 2009.
2. Raghavan, P., *At. Data Nuc. Data Tables*, 42, 189, 1989.
3. Pyykkö, P., *Mol. Phys*. 106, 1965, 2008.
4. Stone, N. J., *At. Data Nucl. Data Tables*, 90, 75, 2005.
5. IUPAC Commission on Physiochemical Symbols, Terminology and Units, *Quantities, Units, and Symbols in Physical Chemistry, Third Edition*, Royal Society of Chemistry, Cambridge, 2007.

		Abundance		ν/MHz for	Relative Sensitivity			
Z	Isotope	%	I	H_0 = 1 T	Const. H_0	Const. ν	μ/μ_N	Q/fm^2
1	^{1}n		1/2	29.1647	0.32139	0.6850	−1.91304272	
1	^{1}H	99.9885	1/2	42.5775	1.00000	1.0000	+2.792847337	
1	^{2}H	0.0115	1	6.5359	0.00965	0.4094	+0.857438228	+0.2860
1	^{3}H	*	1/2	45.4148	1.21354	1.0667	+2.9789625	
2	^{3}He	0.000134	1/2	32.4380	0.44220	0.7619	−2.127750	
3	^{6}Li	7.59	1	6.2661	0.00850	0.3925	+0.8220467	−0.0808
3	^{7}Li	92.41	3/2	16.5483	0.29356	1.9434	+3.25644	−4.01
4	^{9}Be	100	3/2	5.9842	0.01388	0.7028	−1.1776	+5.288
5	^{10}B	19.9	3	4.5752	0.01985	1.7193	+1.800645	+8.459
5	^{11}B	80.1	3/2	13.6630	0.16522	1.6045	+2.688649	+4.059
6	^{13}C	1.07	1/2	10.7084	0.01591	0.2515	+0.7024118	
7	^{14}N	99.636	1	3.0777	0.00101	0.1928	+0.4037610	+2.044
7	^{15}N	0.364	1/2	4.3173	0.00104	0.1014	−0.2831888	
8	^{17}O	0.038	5/2	5.7742	0.02910	1.5822	−1.89379	−2.558
9	^{19}F	100	1/2	40.0776	0.83400	0.9413	+2.628868	
10	^{21}Ne	0.27	3/2	3.3631	0.00246	0.3949	−0.661797	+10.155
11	^{23}Na	100	3/2	11.2688	0.09270	1.3234	+2.217522	+10.4
12	^{25}Mg	10.00	5/2	2.6083	0.00268	0.7147	−0.85545	+19.94
13	^{27}Al	100	5/2	11.1031	0.20689	3.0424	+3.641507	+14.66
14	^{29}Si	4.685	1/2	8.4655	0.00786	0.1988	−0.55529	
15	^{31}P	100	1/2	17.2515	0.06652	0.4052	+1.13160	
16	^{33}S	0.75	3/2	3.2717	0.00227	0.3842	+0.6438212	−6.78
17	^{35}Cl	75.76	3/2	4.1765	0.00472	0.4905	+0.8218743	−8.165
17	^{37}Cl	24.24	3/2	3.4765	0.00272	0.4083	+0.6841236	−6.435
18	^{37}Ar	*	3/2	5.819	0.01276	0.6833	+1.145	+7.6
18	^{39}Ar	*	7/2	3.46	0.01130	1.7080	−1.59	−12
19	^{39}K	93.2581	3/2	1.9893	0.00051	0.2336	+0.3914662	+5.85
19	^{40}K	0.0117	4	2.4737	0.00523	1.5493	−1.298100	−7.3
19	^{41}K	6.7302	3/2	1.0919	0.00008	0.1282	+0.2148701	+7.11

		Abundance		ν/MHz for	Relative Sensitivity			
Z	Isotope	%	I	H_0 = 1 T	Const. H_0	Const. ν	μ/μ$_N$	*Q*/fm^2
20	^{43}Ca	0.135	7/2	2.8697	0.00643	1.4154	−1.317643	−4.08
21	^{45}Sc	100	7/2	10.3591	0.30244	5.1094	+4.756487	−22.0
22	^{47}Ti	7.44	5/2	2.4041	0.00210	0.6588	−0.78848	+30.2
22	^{49}Ti	5.41	7/2	2.4048	0.00378	1.1861	−1.10417	+24.7
23	^{50}V	0.250	6	4.2505	0.05571	5.5905	+3.345689	+21
23	^{51}V	99.750	7/2	11.2133	0.38360	5.5307	+5.1487057	−5.2
24	^{53}Cr	9.501	3/2	2.4115	0.00091	0.2832	−0.47454	−15
25	^{55}Mn	100	5/2	10.5763	0.17881	2.8981	+3.46872	+33
26	^{57}Fe	2.119	1/2	1.3816	0.00003	0.0324	+0.0906230	+16
27	^{59}Co	100	7/2	10.077	0.27841	4.9703	+4.627	+42
28	^{61}Ni	1.1399	3/2	3.8114	0.00359	0.4476	−0.75002	+16.2
29	^{63}Cu	69.15	3/2	11.3188	0.09393	1.3292	+2.2273456	−22.0
29	^{65}Cu	30.85	3/2	12.1027	0.11484	1.4213	+2.38161	−20.4
30	^{67}Zn	4.102	5/2	2.6685	0.00287	0.7312	+0.875205	+15.0
31	^{69}Ga	60.108	3/2	10.2478	0.06971	1.2035	+2.01659	+17.1
31	^{71}Ga	39.892	3/2	13.0208	0.14300	1.5291	+2.56227	+10.7
32	^{73}Ge	7.76	9/2	1.4897	0.00141	1.1547	−0.8794677	−19.6
33	^{75}As	100	3/2	7.3150	0.02536	0.8590	+1.439475	+31.4
34	^{77}Se	7.63	1/2	8.1568	0.00703	0.1916	+0.5350422	
35	^{79}Br	50.69	3/2	10.7042	0.07945	1.2570	+2.106400	+31.3
35	^{81}Br	49.31	3/2	11.5384	0.09951	1.3550	+2.270562	+26.2
36	^{83}Kr	11.500	9/2	1.6442	0.00190	1.2744	−0.970669	+25.9
37	^{85}Rb	72.17	5/2	4.1253	0.01061	1.1304	+1.35298	+27.6
37	^{87}Rb	27.83	3/2	13.9814	0.17704	1.6419	+2.75131	+13.35
38	^{87}Sr	7.00	9/2	1.8525	0.00272	1.4358	−1.093603	+30.5
39	^{89}Y	100	1/2	2.0949	0.00012	0.0492	−0.1374154	
40	^{91}Zr	11.22	5/2	3.9748	0.00949	1.0892	−1.30362	−17.6
41	^{93}Nb	100	9/2	10.4523	0.48821	8.1013	+6.1705	−32
42	^{95}Mo	15.90	5/2	2.7874	0.00327	0.7638	−0.9142	−2.2
42	^{97}Mo	9.56	5/2	2.8463	0.00349	0.7799	−0.9335	+25.5
43	^{99}Tc	*	9/2	9.6294	0.38174	7.4635	+5.6847	−12.9
44	^{99}Ru	12.76	5/2	1.9553	0.00113	0.5358	−0.6413	+7.9
44	^{101}Ru	17.06	5/2	2.1916	0.00159	0.6005	−0.7188	+45.7
45	^{103}Rh	100	1/2	1.3477	0.00003	0.0317	−0.08840	
46	^{105}Pd	22.33	5/2	1.957	0.00113	0.5364	−0.642	+66.0
47	^{107}Ag	51.839	1/2	1.7331	0.00007	0.0407	−0.1136796	
47	^{109}Ag	48.161	1/2	1.9924	0.00010	0.0468	−0.1306906	
48	^{111}Cd	12.80	1/2	9.0692	0.00966	0.2130	−0.5948861	
48	^{113}Cd	12.22	1/2	9.4871	0.01106	0.2228	−0.6223009	
49	^{113}In	4.29	9/2	9.3655	0.35121	7.2589	+5.5289	+75.9
49	^{115}In	95.71	9/2	9.3856	0.35348	7.2745	+5.5408	+77.0
50	^{115}Sn	0.34	1/2	14.0077	0.03561	0.3290	−0.91883	
50	^{117}Sn	7.68	1/2	15.2610	0.04605	0.3584	−1.00104	
50	^{119}Sn	8.59	1/2	15.9660	0.05273	0.3750	−1.04728	
51	^{121}Sb	57.21	5/2	10.2551	0.16302	2.8101	+3.3634	−54.3
51	^{123}Sb	42.79	7/2	5.5532	0.04659	2.7390	+2.5498	−69.2
52	^{123}Te	0.89	1/2	11.2349	0.01837	0.2639	−0.7369478	
52	^{125}Te	7.07	1/2	13.5446	0.03219	0.3181	−0.8884509	
53	^{127}I	100	5/2	8.5778	0.09540	2.3504	+2.813273	−69.6
54	^{129}Xe	26.4006	1/2	11.8604	0.02162	0.2786	−0.7779763	
54	^{131}Xe	21.2324	3/2	3.5159	0.00282	0.4129	+0.6918619	−11.4
55	^{133}Cs	100	7/2	5.6234	0.04838	2.7736	+2.582025	−0.343
56	^{135}Ba	6.592	3/2	4.2617	0.00501	0.5005	+0.838627	+16.0
56	^{137}Ba	11.232	3/2	4.7634	0.00700	0.5594	+0.937365	+24.5
57	^{138}La	0.090	5	5.6615	0.09404	5.3189	+3.713646	+45

		Abundance		ν/MHz for	Relative Sensitivity			
Z	Isotope	%	I	H_0 = 1 T	Const. H_0	Const. ν	μ/μ_N	Q/fm^2
57	^{139}La	99.910	7/2	6.0612	0.06058	2.9895	+2.7830455	+20.0
58	^{137}Ce	*	3/2	4.88	0.00752	0.5729	0.96	
58	^{139}Ce	*	3/2	5.39	0.01012	0.6326	1.06	
58	^{141}Ce	*	7/2	2.37	0.00364	1.1709	1.09	
59	^{141}Pr	100	5/2	13.0359	0.33483	3.5720	+4.2754	−5.9
60	^{143}Nd	12.2	7/2	2.319	0.00339	1.1440	−1.065	−63
60	^{145}Nd	8.3	7/2	1.429	0.00079	0.7047	−0.656	−33
61	^{143}Pm	*	5/2	11.59	0.23510	3.1748	+3.80	
61	^{147}Pm	*	7/2	5.62	0.04827	2.7714	+2.58	+74
62	^{147}Sm	14.99	7/2	1.7748	0.00152	0.8754	−0.8149	−26
62	^{149}Sm	13.82	7/2	1.4631	0.00085	0.7216	−0.6718	+7.4
63	^{151}Eu	47.81	5/2	10.5856	0.17929	2.9006	+3.4718	+90.3
63	^{153}Eu	52.19	5/2	4.6745	0.01544	1.2809	+1.5331	+241
64	^{155}Gd	14.80	3/2	1.312	0.00015	0.1541	−0.2582	+127
64	^{157}Gd	15.65	3/2	1.720	0.00033	0.2020	−0.3385	+135
65	^{159}Tb	100	3/2	10.23	0.06945	1.2019	+2.014	+143.2
66	^{161}Dy	18.889	5/2	1.4654	0.00048	0.4015	−0.4806	+250.7
66	^{163}Dy	24.896	5/2	2.0508	0.00130	0.5619	+0.6726	+265
67	^{165}Ho	100	7/2	9.0883	0.20423	4.4826	+4.173	+358
68	^{167}Er	22.869	7/2	1.2281	0.00050	0.6057	−0.5639	+356.5
69	^{169}Tm	100	1/2	3.531	0.00057	0.0829	−0.2316	−120
70	^{171}Yb	14.28	1/2	7.5261	0.00552	0.1768	+0.49367	
70	^{173}Yb	16.13	5/2	2.0730	0.00135	0.5680	−0.67989	+280
71	^{175}Lu	97.41	7/2	4.8626	0.03128	2.3984	+2.2327	+349
71	^{176}Lu	2.59	7	3.451	0.03975	6.0518	+3.169	+497
72	^{177}Hf	18.60	7/2	1.7282	0.00140	0.8524	+0.7935	+336.5
72	^{179}Hf	13.62	9/2	1.0856	0.00055	0.8414	−0.6409	+379.3
73	^{181}Ta	99.988	7/2	5.1627	0.03744	2.5464	+2.3705	+317
74	^{183}W	14.31	1/2	1.7957	0.00008	0.0422	+0.1177848	
75	^{185}Re	37.40	5/2	9.7176	0.13870	2.6628	+3.1871	+218
75	^{187}Re	62.60	5/2	9.8170	0.14300	2.6900	+3.2197	+207
76	^{187}Os	1.96	1/2	0.9856	0.00001	0.0231	+0.06465189	
76	^{189}Os	16.15	3/2	3.3536	0.00244	0.3938	+0.659933	+85.6
77	^{191}Ir	37.3	3/2	0.7658	0.00003	0.0899	+0.1507	+81.6
77	^{193}Ir	62.7	3/2	0.8319	0.00004	0.0977	+0.1637	+75.1
78	^{195}Pt	33.832	1/2	9.2922	0.01039	0.2182	+0.60952	
79	^{197}Au	100	3/2	0.7406	0.00003	0.0870	+0.145746	+54.7
80	^{199}Hg	16.87	1/2	7.7123	0.00594	0.1811	+0.5058855	
80	^{201}Hg	13.18	3/2	2.8469	0.00149	0.3343	−0.5602257	+38.7
81	^{203}Tl	29.52	1/2	24.7316	0.19598	0.5809	+1.6222579	
81	^{205}Tl	70.48	1/2	24.9749	0.20182	0.5866	+1.6382146	
82	^{207}Pb	22.1	1/2	9.0340	0.00955	0.2122	+0.59258	
83	^{209}Bi	100	9/2	6.9630	0.14433	5.3968	+4.1106	−51.6
84	^{209}Po	*	1/2	11.7	0.02096	0.2757	+0.77	
86	^{211}Rn	*	1/2	9.16	0.00997	0.2152	+0.601	
87	^{223}Fr	*	3/2	5.95	0.01362	0.6982	+1.17	+117
88	^{223}Ra	*	3/2	1.3746	0.00017	0.1614	+0.2705	+121
88	^{225}Ra	*	1/2	11.187	0.01814	0.2627	−0.7338	
89	^{227}Ac	*	3/2	5.6	0.01131	0.6565	+1.1	+170
90	^{229}Th	*	5/2	1.40	0.00042	0.3843	+0.46	+430
91	^{231}Pa	100	3/2	10.2	0.06903	1.1995	2.01	−172
92	^{235}U	0.7204	7/2	0.83	0.00015	0.4082	−0.38	+493.6
93	^{237}Np	*	5/2	9.57	0.13264	2.6234	+3.14	+388.6
94	^{239}Pu	*	1/2	3.09	0.00038	0.0727	+0.203	
95	^{243}Am	*	5/2	4.6	0.01446	1.2532	+1.5	+421