

Isotope	Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla)											
			Natural rel. ¹³ C	Molar rel. ¹ H	Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments											
					7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904	
1	H	1/2	99.9885	5.87E+03	1.00E+00	300.130	400.130	500.130	600.130	700.130	750.130	800.130	850.130	900.130	950.130	1000.130
2	H	1	0.0115	6.52E-03	9.65E-03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
3	H	1/2		-	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
3	He	1/2	1.34E-04	3.48E-03	4.42E-01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
6	Li	1	7.59	3.79E+00	8.50E-03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
7	Li	3/2	92.41	1.59E+03	2.94E-01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
9	Be	3/2	100.0	8.15E+01	1.39E-02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
10	B	3	19.9	2.32E+01	1.99E-02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
11	B	3/2	80.1	7.77E+02	1.65E-01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.757	288.797	304.839	320.881
13	C	1/2	1.07	1.00E+00	1.59E-02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
14	N	1	99.636	5.90E+00	1.01E-03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
15	N	1/2	0.364	2.23E-02	1.04E-03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
17	O	5/2	0.038	6.50E-02	2.91E-02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
19	F	1/2	100.0	4.89E+03	8.32E-01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
21	Ne	3/2	0.27	3.91E-02	2.46E-03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
23	Na	3/2	100.0	5.45E+02	9.27E-02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
25	Mg	5/2	10.00	1.58E+00	2.68E-03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
27	Al	5/2	100.0	1.22E+03	2.07E-01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
29	Si	1/2	4.685	2.16E+00	7.86E-03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
31	P	1/2	100.0	3.91E+02	6.65E-02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
33	S	3/2	0.75	1.00E-01	2.27E-03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
35	Cl	3/2	75.76	2.10E+01	4.72E-03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
37	Cl	3/2	24.24	3.88E+00	2.72E-03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
39	K	3/2	93.258	2.79E+00	5.10E-04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
41	K	3/2	6.730	3.34E-02	8.44E-05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
43	Ca	7/2	0.135	5.10E-02	6.43E-03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309
45	Sc	7/2	100.0	1.78E+03	3.02E-01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
47	Ti	5/2	7.44	9.18E-01	2.10E-03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
49	Ti	7/2	5.41	1.20E+00	3.78E-03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
50	V	6	0.250	8.18E-01	5.57E-02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
51	V	7/2	99.750	2.25E+03	3.84E-01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
53	Cr	3/2	9.501	5.07E-01	9.08E-04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
55	Mn	5/2	100.0	1.05E+03	1.79E-01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
57	Fe	1/2	2.119	4.25E-03	3.42E-05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
59	Co	7/2	100.0	1.64E+03	2.78E-01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
61	Ni	3/2	1.1399	2.40E-01	3.59E-03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
63	Cu	3/2	69.15	3.82E+02	9.39E-02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
65	Cu	3/2	30.85	2.08E+02	1.15E-01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
67	Zn	5/2	4.102	6.92E-01	2.87E-03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
69	Ga	3/2	60.108	2.46E+02	6.97E-02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
71	Ga	3/2	39.892	3.35E+02	1.43E-01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007

NMR Frequency Tables



NMR Frequencies vs. Bruker Field Strengths – sorted by increasing atomic number

Isotope	Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla)											
			Natural rel. ¹³ C	Molar rel. ¹ H	Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments											
					7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904	
73	Ge	9/2	7.76	6.44E-01	1.41E-03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
75	As	3/2	100.0	1.49E+02	2.54E-02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
77	Se	1/2	7.63	3.15E+00	7.03E-03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
79	Br	3/2	50.69	2.37E+02	7.94E-02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
81	Br	3/2	49.31	2.88E+02	9.95E-02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
83	Kr	9/2	11.500	1.28E+00	1.90E-03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
85	Rb	5/2	72.17	4.50E+01	1.06E-02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
87	Rb	3/2	27.83	2.90E+02	1.77E-01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
87	Sr	9/2	7.00	1.12E+00	2.72E-03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
89	Y	1/2	100.0	7.00E-01	1.19E-04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
91	Zr	5/2	11.22	6.26E+00	9.49E-03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
93	Nb	9/2	100.0	2.87E+03	4.88E-01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
95	Mo	5/2	15.90	3.06E+00	3.27E-03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
97	Mo	5/2	9.56	1.96E+00	3.49E-03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
99	Tc	9/2	-	-	3.82E-01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
99	Ru	5/2	12.76	8.46E-01	1.13E-03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
101	Ru	5/2	17.06	1.58E+00	1.57E-03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
103	Rh	1/2	100.0	1.86E-01	3.17E-05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
105	Pd	5/2	22.33	1.49E+00	1.13E-03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
107	Ag	1/2	51.839	2.05E-01	6.74E-05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
109	Ag	1/2	48.161	2.90E-01	1.02E-04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
111	Cd	1/2	12.80	7.27E+00	9.66E-03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
113	Cd	1/2	12.22	7.94E+00	1.11E-02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
113	In	9/2	4.29	8.85E+01	3.51E-01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
115	In	9/2	95.71	1.99E+03	3.53E-01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155
115	Sn	1/2	0.34	7.11E-01	3.56E-02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
117	Sn	1/2	7.68	2.08E+01	4.60E-02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
119	Sn	1/2	8.59	2.66E+01	5.27E-02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
121	Sb	5/2	57.21	5.48E+02	1.63E-01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
123	Sb	7/2	42.79	1.17E+02	4.66E-02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
123	Te	1/2	0.89	9.61E-01	1.84E-02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
125	Te	1/2	7.07	1.34E+01	3.22E-02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
127	I	5/2	100.0	5.60E+02	9.54E-02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
129	Xe	1/2	26.4006	3.35E+01	2.16E-02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
131	Xe	3/2	21.2324	3.51E+00	2.82E-03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
133	Cs	7/2	100.0	2.84E+02	4.84E-02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
135	Ba	3/2	6.592	1.94E+00	5.01E-03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
137	Ba	3/2	11.232	4.62E+00	7.00E-03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
138	La	5	0.090	4.97E-01	9.40E-02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
139	La	7/2	99.910	3.56E+02	6.06E-02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
141	Pr	5/2	100.0	1.97E+03	3.35E-01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21

NMR Frequency Tables



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						7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
143	Nd	7/2	12.2	2.43E+00	3.39E-03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
145	Nd	7/2	8.3	3.87E-01	7.93E-04	10.07	13.43	17.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
147	Sm	7/2	14.99	1.34E+00	1.52E-03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
149	Sm	7/2	13.82	6.92E-01	8.52E-04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
151	Eu	5/2	47.81	5.04E+02	1.79E-01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
153	Eu	5/2	52.19	4.73E+01	1.54E-02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
155	Gd	3/2	14.80	1.26E-01	1.45E-04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
157	Gd	3/2	15.65	3.00E-01	3.26E-04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
159	Tb	3/2	100.0	4.08E+02	6.94E-02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
161	Dy	5/2	18.889	5.26E-01	4.74E-04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
163	Dy	5/2	24.896	1.91E+00	1.31E-03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
165	Ho	7/2	100.0	1.16E+03	1.98E-01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
167	Er	7/2	22.869	6.77E-01	5.04E-04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
169	Tm	1/2	100.0	3.32E+00	5.66E-04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
171	Yb	1/2	14.28	4.63E+00	5.52E-03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
173	Yb	5/2	16.13	1.28E+00	1.35E-03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
175	Lu	7/2	97.41	1.79E+02	3.13E-02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
176	Lu	7	2.59	6.05E+00	3.98E-02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
177	Hf	7/2	18.60	1.53E+00	1.40E-03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
179	Hf	9/2	13.62	4.38E-01	5.47E-04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
181	Ta	7/2	99.988	2.20E+02	3.74E-02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
183	W	1/2	14.31	6.31E-02	7.50E-05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
185	Re	5/2	37.40	3.05E+02	1.39E-01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
187	Re	5/2	62.60	5.26E+02	1.43E-01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
187	Os	1/2	1.96	1.43E-03	1.24E-05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
189	Os	3/2	16.15	2.32E+00	2.44E-03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
191	Ir	3/2	37.3	6.38E-02	2.91E-05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
193	Ir	3/2	62.7	1.37E-01	3.73E-05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
195	Pt	1/2	33.832	2.07E+01	1.04E-02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
197	Au	3/2	100.0	1.62E-01	2.76E-05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69
199	Hg	1/2	16.87	5.89E+00	5.94E-03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
201	Hg	3/2	13.18	1.16E+00	1.49E-03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
203	Tl	1/2	29.52	3.40E+02	1.96E-01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
205	Tl	1/2	70.48	8.36E+02	2.02E-01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
207	Pb	1/2	22.1	1.18E+01	9.06E-03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
209	Bi	9/2	100.0	8.48E+02	1.44E-01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
209	Po	1/2		-	1.44E-02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
231	Pa	3/2	100.0	4.06E+02	6.90E-02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
235	U	7/2	0.7204	6.53E-03	1.54E-04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416

NMR Frequency Tables



NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope	Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla)										
			Natural rel. ¹³ C	Molar rel. ¹ H	Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
					7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
3 H	1/2		–	1.21E+00	320.131	426.795	533.459	640.123	746.786	800.118	853.450	906.782	960.114	1013.446	1066.778
1 H	1/2	99.9885	5.87E+03	1.00E+00	300.130	400.130	500.130	600.130	700.130	750.130	800.130	850.130	900.130	950.130	1000.130
19 F	1/2	100.0	4.89E+03	8.32E–01	282.404	376.498	470.592	564.686	658.780	705.827	752.874	799.921	846.968	894.015	941.062
3 He	1/2	1.34E–04	3.48E–03	4.42E–01	228.636	304.815	380.994	457.173	533.352	571.441	609.531	647.620	685.710	723.799	761.889
205 Tl	1/2	70.48	8.36E+02	2.02E–01	173.127	230.810	288.494	346.178	403.862	432.704	461.546	490.388	519.230	548.071	576.913
203 Tl	1/2	29.52	3.40E+02	1.96E–01	171.444	228.567	285.690	342.813	399.937	428.498	457.060	485.621	514.183	542.745	571.306
31 P	1/2	100.0	3.91E+02	6.65E–02	121.495	161.976	202.457	242.938	283.419	303.659	323.900	344.140	364.380	384.621	404.861
7 Li	3/2	92.41	1.59E+03	2.94E–01	116.642	155.506	194.370	233.233	272.097	291.529	310.961	330.393	349.825	369.257	388.688
119 Sn	1/2	8.59	2.66E+01	5.27E–02	111.920	149.211	186.502	223.792	261.083	279.728	298.374	317.019	335.664	354.309	372.955
117 Sn	1/2	7.68	2.08E+01	4.60E–02	106.943	142.575	178.208	213.840	249.472	267.288	285.104	302.921	320.737	338.553	356.369
87 Rb	3/2	27.83	2.90E+02	1.77E–01	98.204	130.924	163.645	196.365	229.086	245.446	261.806	278.166	294.527	310.887	327.247
115 Sn	1/2	0.34	7.11E–01	3.56E–02	98.199	130.918	163.636	196.355	229.074	245.433	261.793	278.152	294.511	310.871	327.230
11 B	3/2	80.1	7.77E+02	1.65E–01	96.294	128.378	160.462	192.546	224.630	240.672	256.714	272.755	288.797	304.839	320.881
125 Te	1/2	7.07	1.34E+01	3.22E–02	94.690	126.240	157.790	189.340	220.889	236.664	252.439	268.214	283.989	299.764	315.539
141 Pr	5/2	100.0	1.97E+03	3.35E–01	91.89	122.51	153.12	183.74	214.36	229.67	244.97	260.28	275.59	290.90	306.21
71 Ga	3/2	39.892	3.35E+02	1.43E–01	91.530	122.026	152.523	183.020	213.517	228.765	244.013	259.262	274.510	289.758	305.007
65 Cu	3/2	30.85	2.08E+02	1.15E–01	85.248	113.652	142.055	170.459	198.863	213.065	227.266	241.468	255.670	269.872	284.074
129 Xe	1/2	26.4006	3.35E+01	2.16E–02	83.467	111.277	139.087	166.897	194.707	208.613	222.518	236.423	250.328	264.233	278.138
81 Br	3/2	49.31	2.88E+02	9.95E–02	81.055	108.061	135.068	162.074	189.081	202.584	216.087	229.591	243.094	256.597	270.100
63 Cu	3/2	69.15	3.82E+02	9.39E–02	79.581	106.096	132.612	159.127	185.643	198.901	212.158	225.416	238.674	251.931	265.189
23 Na	3/2	100.0	5.45E+02	9.27E–02	79.390	105.842	132.294	158.746	185.198	198.424	211.650	224.876	238.101	251.327	264.553
51 V	7/2	99.750	2.25E+03	3.84E–01	78.943	105.246	131.549	157.852	184.155	197.306	210.458	223.609	236.761	249.912	263.064
123 Te	1/2	0.89	9.61E–01	1.84E–02	78.543	104.713	130.883	157.052	183.222	196.307	209.392	222.477	235.562	248.647	261.731
27 Al	5/2	100.0	1.22E+03	2.07E–01	78.204	104.261	130.318	156.375	182.432	195.460	208.489	221.517	234.546	247.574	260.602
13 C	1/2	1.07	1.00E+00	1.59E–02	75.468	100.613	125.758	150.903	176.048	188.620	201.193	213.765	226.338	238.910	251.483
79 Br	3/2	50.69	2.37E+02	7.94E–02	75.195	100.248	125.302	150.356	175.410	187.937	200.464	212.991	225.518	238.045	250.572
151 Eu	5/2	47.81	5.04E+02	1.79E–01	74.62	99.48	124.34	149.20	174.06	186.49	198.92	211.35	223.78	236.22	248.65
55 Mn	5/2	100.0	1.05E+03	1.79E–01	74.400	99.189	123.978	148.768	173.557	185.951	198.346	210.741	223.135	235.530	247.924
93 Nb	9/2	100.0	2.87E+03	4.88E–01	73.460	97.936	122.413	146.889	171.365	183.603	195.841	208.079	220.317	232.555	244.794
209 Po	1/2		–	1.44E–02	73.08	97.42	121.77	146.12	170.47	182.64	194.81	206.99	219.16	231.34	243.51
45 Sc	7/2	100.0	1.78E+03	3.02E–01	72.907	97.199	121.490	145.782	170.074	182.220	194.366	206.511	218.657	230.803	242.949
159 Tb	3/2	100.0	4.08E+02	6.94E–02	72.14	96.18	120.22	144.26	168.29	180.31	192.33	204.35	216.37	228.39	240.41
69 Ga	3/2	60.108	2.46E+02	6.97E–02	72.035	96.037	120.038	144.039	168.041	180.041	192.042	204.043	216.043	228.044	240.045
231 Pa	3/2	100.0	4.06E+02	6.90E–02	72.00	95.99	119.98	143.97	167.96	179.96	191.95	203.94	215.94	227.93	239.93
121 Sb	5/2	57.21	5.48E+02	1.63E–01	71.823	95.753	119.684	143.615	167.545	179.510	191.476	203.441	215.406	227.372	239.337
59 Co	7/2	100.0	1.64E+03	2.78E–01	71.212	94.939	118.666	142.393	166.120	177.984	189.847	201.711	213.575	225.438	237.302
187 Re	5/2	62.60	5.26E+02	1.43E–01	68.284	91.036	113.788	136.539	159.291	170.667	182.042	193.418	204.794	216.170	227.546
185 Re	5/2	37.40	3.05E+02	1.39E–01	67.603	90.128	112.652	135.177	157.701	168.964	180.226	191.488	202.751	214.013	225.275
99 Tc	9/2		–	3.82E–01	67.554	90.063	112.571	135.079	157.588	168.842	180.096	191.350	202.604	213.858	225.113
113 Cd	1/2	12.22	7.94E+00	1.11E–02	66.608	88.802	110.995	133.188	155.381	166.478	177.574	188.671	199.767	210.864	221.961
115 In	9/2	95.71	1.99E+03	3.53E–01	65.766	87.679	109.592	131.504	153.417	164.373	175.330	186.286	197.242	208.198	219.155

Isotope	Spin	Nat. Abund. (%)	Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla)													
			Receptivity		Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments											
			Natural rel. ¹³ C	Molar rel. ¹ H	7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904	
113	In	9/2	4.29	8.85E+01	3.51E-01	65.626	87.491	109.357	131.223	153.089	164.022	174.954	185.887	196.820	207.753	218.686
195	Pt	1/2	33.832	2.07E+01	1.04E-02	64.518	86.015	107.512	129.009	150.505	161.254	172.002	182.751	193.499	204.247	214.996
111	Cd	1/2	12.80	7.27E+00	9.66E-03	63.674	84.890	106.105	127.320	148.536	159.144	169.751	180.359	190.967	201.575	212.182
165	Ho	7/2	100.0	1.16E+03	1.98E-01	63.43	84.57	105.71	126.84	147.98	158.54	169.11	179.68	190.25	200.82	211.38
207	Pb	1/2	22.1	1.18E+01	9.06E-03	62.789	83.710	104.630	125.551	146.471	156.932	167.392	177.852	188.313	198.773	209.233
127	I	5/2	100.0	5.60E+02	9.54E-02	60.048	80.056	100.063	120.071	140.078	150.082	160.086	170.090	180.093	190.097	200.101
29	Si	1/2	4.685	2.16E+00	7.86E-03	59.627	79.495	99.362	119.229	139.096	149.030	158.963	168.897	178.831	188.764	198.698
77	Se	1/2	7.63	3.15E+00	7.03E-03	57.239	76.311	95.382	114.454	133.525	143.061	152.597	162.133	171.668	181.204	190.740
199	Hg	1/2	16.87	5.89E+00	5.94E-03	53.756	71.667	89.577	107.488	125.399	134.354	143.310	152.265	161.221	170.176	179.132
171	Yb	1/2	14.28	4.63E+00	5.52E-03	52.521	70.020	87.519	105.019	122.518	131.268	140.017	148.767	157.517	166.266	175.016
75	As	3/2	100.0	1.49E+02	2.54E-02	51.390	68.513	85.635	102.758	119.881	128.442	137.003	145.564	154.126	162.687	171.248
209	Bi	9/2	100.0	8.48E+02	1.44E-01	48.229	64.298	80.367	96.437	112.506	120.541	128.575	136.610	144.644	152.679	160.714
2	H	1	0.0115	6.52E-03	9.65E-03	46.072	61.422	76.773	92.124	107.474	115.150	122.825	130.500	138.175	145.851	153.526
6	Li	1	7.59	3.79E+00	8.50E-03	44.167	58.883	73.600	88.316	103.032	110.390	117.748	125.106	132.464	139.822	147.180
139	La	7/2	99.910	3.56E+02	6.06E-02	42.395	56.521	70.647	84.772	98.898	105.961	113.023	120.086	127.149	134.212	141.275
9	Be	3/2	100.0	8.15E+01	1.39E-02	42.174	56.226	70.277	84.329	98.381	105.407	112.433	119.459	126.485	133.510	140.536
17	O	5/2	0.038	6.50E-02	2.91E-02	40.687	54.243	67.800	81.356	94.913	101.691	108.469	115.248	122.026	128.804	135.582
138	La	5	0.090	4.97E-01	9.40E-02	39.600	52.794	65.989	79.183	92.377	98.974	105.572	112.169	118.766	125.363	131.960
133	Cs	7/2	100.0	2.84E+02	4.84E-02	39.365	52.482	65.598	78.714	91.830	98.388	104.946	111.504	118.062	124.620	131.178
123	Sb	7/2	42.79	1.17E+02	4.66E-02	38.894	51.854	64.813	77.772	90.731	97.211	103.691	110.170	116.650	123.129	129.609
181	Ta	7/2	99.988	2.20E+02	3.74E-02	35.984	47.974	59.964	71.953	83.943	89.938	95.932	101.927	107.922	113.917	119.912
175	Lu	7/2	97.41	1.79E+02	3.13E-02	34.27	45.69	57.11	68.53	79.94	85.65	91.36	97.07	102.78	108.49	114.20
137	Ba	3/2	11.232	4.62E+00	7.00E-03	33.353	44.466	55.579	66.692	77.805	83.361	88.918	94.474	100.031	105.587	111.144
153	Eu	5/2	52.19	4.73E+01	1.54E-02	32.94	43.91	54.88	65.86	76.83	82.32	87.80	93.29	98.78	104.26	109.75
10	B	3	19.9	2.32E+01	1.99E-02	32.245	42.989	53.732	64.476	75.220	80.591	85.963	91.335	96.707	102.079	107.451
15	N	1/2	0.364	2.23E-02	1.04E-03	30.423	40.560	50.697	60.834	70.971	76.039	81.107	86.176	91.244	96.312	101.381
50	V	6	0.250	8.18E-01	5.57E-02	29.924	39.894	49.865	59.835	69.805	74.790	79.775	84.761	89.746	94.731	99.716
135	Ba	3/2	6.592	1.94E+00	5.01E-03	29.816	39.751	49.685	59.620	69.554	74.521	79.489	84.456	89.423	94.390	99.357
35	Cl	3/2	75.76	2.10E+01	4.72E-03	29.406	39.204	49.002	58.800	68.598	73.497	78.396	83.295	88.194	93.093	97.992
85	Rb	5/2	72.17	4.50E+01	1.06E-02	28.977	38.632	48.287	57.942	67.597	72.425	77.252	82.080	86.907	91.735	96.562
91	Zr	5/2	11.22	6.26E+00	9.49E-03	27.901	37.197	46.494	55.790	65.086	69.734	74.382	79.031	83.679	88.327	92.975
61	Ni	3/2	1.1399	2.40E-01	3.59E-03	26.820	35.756	44.692	53.628	62.564	67.032	71.500	75.968	80.436	84.904	89.372
169	Tm	1/2	100.0	3.32E+00	5.66E-04	24.82	33.10	41.37	49.64	57.91	62.04	66.18	70.32	74.45	78.59	82.72
131	Xe	3/2	21.2324	3.51E+00	2.82E-03	24.742	32.986	41.230	49.474	57.718	61.840	65.962	70.084	74.206	78.328	82.450
37	Cl	3/2	24.24	3.88E+00	2.72E-03	24.478	32.634	40.789	48.945	57.101	61.179	65.256	69.334	73.412	77.490	81.568
176	Lu	7	2.59	6.05E+00	3.98E-02	24.33	32.43	40.53	48.64	56.74	60.80	64.85	68.90	72.95	77.01	81.06
21	Ne	3/2	0.27	3.91E-02	2.46E-03	23.693	31.587	39.482	47.376	55.270	59.217	63.165	67.112	71.059	75.006	78.953
189	Os	3/2	16.15	2.32E+00	2.44E-03	23.306	31.072	38.837	46.602	54.368	58.251	62.133	66.016	69.899	73.781	77.664
33	S	3/2	0.75	1.00E-01	2.27E-03	23.038	30.714	38.390	46.066	53.742	57.580	61.418	65.256	69.094	72.932	76.770
14	N	1	99.636	5.90E+00	1.01E-03	21.688	28.915	36.141	43.367	50.594	54.207	57.820	61.433	65.046	68.659	72.273
43	Ca	7/2	0.135	5.10E-02	6.43E-03	20.199	26.929	33.659	40.389	47.119	50.484	53.849	57.214	60.579	63.944	67.309

NMR Frequency Tables



NMR Frequencies vs. Bruker Field Strengths – sorted with decreasing Larmor frequency

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla)										
				Natural rel. ¹³ C	Molar rel. ¹ H	Freq. to 3 decimals are experimental for IUPAC Standards; freq. to 2 dec. are calculated from magn. moments										
						7.04925	9.39798	11.7467	14.0954	16.4442	17.6185	18.7929	19.9673	21.1416	22.3160	23.4904
97	Mo	5/2	9.56	1.96E+00	3.49E-03	19.970	26.623	33.277	39.931	46.585	49.911	53.238	56.565	59.892	63.219	66.546
201	Hg	3/2	13.18	1.16E+00	1.49E-03	19.843	26.455	33.067	39.678	46.290	49.595	52.901	56.207	59.513	62.819	66.124
95	Mo	5/2	15.90	3.06E+00	3.27E-03	19.559	26.076	32.593	39.110	45.627	48.885	52.144	55.402	58.661	61.919	65.178
67	Zn	5/2	4.102	6.92E-01	2.87E-03	18.779	25.035	31.292	37.549	43.806	46.934	50.063	53.191	56.319	59.448	62.576
25	Mg	5/2	10.00	1.58E+00	2.68E-03	18.373	24.494	30.616	36.738	42.859	45.920	48.981	52.042	55.103	58.163	61.224
53	Cr	3/2	9.501	5.07E-01	9.08E-04	16.965	22.617	28.270	33.922	39.575	42.401	45.227	48.054	50.880	53.706	56.532
49	Ti	7/2	5.41	1.20E+00	3.78E-03	16.924	22.563	28.203	33.842	39.481	42.300	45.120	47.939	50.759	53.578	56.398
47	Ti	5/2	7.44	9.18E-01	2.10E-03	16.920	22.557	28.195	33.833	39.470	42.289	45.108	47.926	50.745	53.564	56.383
143	Nd	7/2	12.2	2.43E+00	3.39E-03	16.35	21.80	27.25	32.69	38.14	40.86	43.59	46.31	49.04	51.76	54.48
101	Ru	5/2	17.06	1.58E+00	1.57E-03	15.491	20.652	25.814	30.975	36.136	38.717	41.298	43.878	46.459	49.040	51.620
89	Y	1/2	100.0	7.00E-01	1.19E-04	14.707	19.607	24.507	29.408	34.308	36.758	39.208	41.658	44.108	46.558	49.008
173	Yb	5/2	16.13	1.28E+00	1.35E-03	14.61	19.48	24.35	29.22	34.09	36.52	38.96	41.39	43.83	46.26	48.69
163	Dy	5/2	24.896	1.91E+00	1.31E-03	14.46	19.28	24.10	28.92	33.74	36.15	38.56	40.97	43.38	45.79	48.20
39	K	3/2	93.258	2.79E+00	5.10E-04	14.005	18.672	23.338	28.004	32.671	35.004	37.337	39.670	42.003	44.337	46.670
109	Ag	1/2	48.161	2.90E-01	1.02E-04	13.967	18.620	23.274	27.927	32.581	34.908	37.234	39.561	41.888	44.215	46.541
99	Ru	5/2	12.76	8.46E-01	1.13E-03	13.821	18.427	23.032	27.637	32.242	34.545	36.847	39.150	41.452	43.755	46.057
105	Pd	5/2	22.33	1.49E+00	1.13E-03	13.734	18.310	22.886	27.463	32.039	34.327	36.615	38.903	41.191	43.479	45.767
87	Sr	9/2	7.00	1.12E+00	2.72E-03	13.007	17.341	21.675	26.009	30.342	32.509	34.676	36.843	39.010	41.177	43.344
147	Sm	7/2	14.99	1.34E+00	1.52E-03	12.51	16.68	20.84	25.01	29.18	31.26	33.35	35.43	37.52	39.60	41.68
183	W	1/2	14.31	6.31E-02	7.50E-05	12.505	16.671	20.837	25.004	29.170	31.253	33.337	35.420	37.503	39.586	41.669
177	Hf	7/2	18.60	1.53E+00	1.40E-03	12.18	16.24	20.30	24.36	28.42	30.45	32.48	34.51	36.53	38.56	40.59
107	Ag	1/2	51.839	2.05E-01	6.74E-05	12.149	16.197	20.244	24.292	28.340	30.364	32.388	34.412	36.436	38.460	40.483
157	Gd	3/2	15.65	3.00E-01	3.26E-04	12.08	16.11	20.13	24.16	28.19	30.20	32.21	34.22	36.24	38.25	40.26
83	Kr	9/2	11.500	1.28E+00	1.90E-03	11.548	15.395	19.243	23.091	26.938	28.862	30.786	32.710	34.633	36.557	38.481
73	Ge	9/2	7.76	6.44E-01	1.41E-03	10.469	13.958	17.446	20.934	24.423	26.167	27.911	29.655	31.399	33.144	34.888
161	Dy	5/2	18.889	5.26E-01	4.74E-04	10.32	13.75	17.19	20.63	24.07	25.78	27.50	29.22	30.94	32.66	34.38
149	Sm	7/2	13.82	6.92E-01	8.52E-04	10.31	13.75	17.18	20.62	24.06	25.77	27.49	29.21	30.93	32.64	34.36
145	Nd	7/2	8.3	3.87E-01	7.93E-04	10.07	13.43	16.78	20.14	23.49	25.17	26.85	28.53	30.20	31.88	33.56
57	Fe	1/2	2.119	4.25E-03	3.42E-05	9.718	12.955	16.193	19.431	22.669	24.288	25.906	27.525	29.144	30.763	32.382
103	Rh	1/2	100.0	1.86E-01	3.17E-05	9.563	12.750	15.936	19.123	22.309	23.902	25.496	27.089	28.682	30.275	31.869
155	Gd	3/2	14.80	1.26E-01	1.45E-04	9.21	12.28	15.35	18.42	21.49	23.03	24.56	26.10	27.63	29.17	30.70
167	Er	7/2	22.869	6.77E-01	5.04E-04	8.66	11.54	14.42	17.31	20.19	21.63	23.08	24.52	25.96	27.40	28.85
41	K	3/2	6.730	3.34E-02	8.44E-05	7.687	10.249	12.810	15.371	17.932	19.213	20.494	21.774	23.055	24.336	25.616
179	Hf	9/2	13.62	4.38E-01	5.47E-04	7.65	10.20	12.75	15.30	17.85	19.13	20.40	21.68	22.95	24.23	25.50
187	Os	1/2	1.96	1.43E-03	1.24E-05	6.850	9.132	11.415	13.697	15.979	17.120	18.262	19.403	20.544	21.685	22.826
193	Ir	3/2	62.7	1.37E-01	3.73E-05	5.86	7.82	9.77	11.73	13.68	14.66	15.63	16.61	17.59	18.56	19.54
235	U	7/2	0.7204	6.53E-03	1.54E-04	5.527	7.368	9.209	11.051	12.892	13.813	14.734	15.654	16.575	17.496	18.416
191	Ir	3/2	37.3	6.38E-02	2.91E-05	5.40	7.20	9.00	10.79	12.59	13.49	14.39	15.29	16.19	17.09	17.99
197	Au	3/2	100.0	1.62E-01	2.76E-05	5.31	7.08	8.84	10.61	12.38	13.26	14.15	15.03	15.92	16.80	17.69

NMR Properties of Selected Isotopes



Z = proton number, **A** = mass number, **Half-Life** where appropriate in years (y), days (d), hours (h), minutes (m); **I** = spin quantum number; **NA** = natural abundance (IUPAC 2003); **μ_z** = z-component of nuclear magnetic moment in units of the nuclear magneton (μ_N); **Q** = electric quadrupole moment in units of fm² = 10⁻³⁰ m² (1 fm² = 0.01 barns); calc. magnetogyric ratio $\gamma = \mu_z/\hbar I$. Note: for **μ_z** and **Q** the experimental uncertainty begins with the last significant digit.

			Isotope (half-life)	Spin	Nat. Abund. 2003 (TICE 2001)	Rel. Nucl. Magn. Mom. (measured)	Quadrupole Moment	Magnetogyric Ratio (calc., free atom)
Z	A	Sym	Name	I	NA (%)	μ_z / μ_N	Q [fm ²]	γ [10 ⁷ rad s ⁻¹ T ⁻¹]
0	1	n	Neutron	1/2		-1.9130427		-18.3247183
1	1	H	Hydrogen	1/2	99.9885	2.79284734		26.7522208
	2	H (D)	Deuterium	1	0.0115	0.857438228	0.286	4.10662919
	3	H (T)	Tritium (12.32 y)	1/2		2.97896244		28.5349865
2	3	He	Helium	1/2	0.000134	-2.12749772		-20.3789473
3	6	Li	Lithium	1	7.59	0.8220473	-0.0808	3.937127
	7	Li	Lithium	3/2	92.41	3.2564625	-4.01	10.397704
4	9	Be	Beryllium	3/2	100	-1.17749	5.288	-3.75966
5	10	B	Boron	3	19.9	1.80064478	8.459	2.87467955
	11	B	Boron	3/2	80.1	2.688649	4.059	8.584707
6	13	C	Carbon	1/2	1.07	0.702412		6.728286
7	14	N	Nitrogen	1	99.636	0.40376100	2.044	1.9337798
	15	N	Nitrogen	1/2	0.364	-0.28318884		-2.7126189
8	17	O	Oxygen	5/2	0.038	-1.89379	-2.558	-3.62806
9	19	F	Fluorine	1/2	100	2.626868		25.16233
10	21	Ne	Neon	3/2	0.27	-0.661797	10.155	-2.113081
11	23	Na	Sodium (Natrium)	3/2	100	2.2176556	10.4	7.0808516
12	25	Mg	Magnesium	5/2	10.00	-0.85545	19.94	-1.63884
13	26	Al	Alumin(i)um (7.17E5 y)	5		2.804	27	2.686
13	27	Al	Alumin(i)um	5/2	100	3.6415069	14.66	6.9762780
14	29	Si	Silicon	1/2	4.685	-0.55529	19.94	-5.31903
15	31	P	Phosphorus	1/2	100	1.13160		10.8394
16	33	S	Sulfur	3/2	0.75	0.643821	-6.78	2.055685
17	35	Cl	Chlorine	3/2	75.76	0.8218743	-8.165	2.6241991
	37	Cl	Chlorine	3/2	24.24	0.6841236	-6.435	2.1843688
18	39	Ar	Argon (269 y)	7/2		-1.59		-2.17
19	39	K	Potassium (Kalium)	3/2	93.258	0.3915073	5.85	1.2500612
	40	K	Potassium (1.248E9 y)	4	0.0117	-1.298100	-7.3	-1.554286
	41	K	Potassium	3/2	6.730	0.21489274	7.11	0.68614062
20	41	Ca	Calcium (1.02E5 y)	7/2		-1.594781	-6.7	-2.182306
	43	Ca	Calcium	7/2	0.135	-1.317643	-4.08	-1.803069
21	45	Sc	Scandium	7/2	100	4.756487	-22.0	6.508800
22	47	Ti	Titanium	5/2	7.44	-0.78848	30.2	-1.51054
	49	Ti	Titanium	7/2	5.41	-1.10417	24.7	-1.51095
23	50	V	Vanadium (1.4E17 y)	6	0.250	3.345689	21	2.670650
	51	V	Vanadium	7/2	99.750	5.1487057	-5.2	7.0455139
24	53	Cr	Chromium	3/2	9.501	-0.47454	-15	-1.51518
25	53	Mn	Manganese (3.74E6 y)	7/2		5.024		6.875
	55	Mn	Manganese	5/2	100	3.46871790	33	6.64525453
26	57	Fe	Iron, Ferrum	1/2	2.119	0.09062300		0.8680627
	59	Fe	Iron (44.507 d)	3/2		-0.3358		-1.0722
27	59	Co	Cobalt	7/2	100	4.627	42 s	6.332
	60	Co	Cobalt (1925.2 d)	5		3.799	44	3.639
28	61	Ni	Nickel	3/2	1.1399	-0.75002	16.2	-2.39477
29	63	Cu	Copper, Cuprum	3/2	69.15	2.227346	-22.0	7.111791
	65	Cu	Copper, Cuprum	3/2	30.85	2.3816	-20.4	7.6043
30	67	Zn	Zinc	5/2	4.102	0.8752049	15.0	1.6766885
31	69	Ga	Gallium	3/2	60.108	2.01659	17.1	6.43886
	71	Ga	Gallium	3/2	39.892	2.56227	10.7	8.18117
32	73	Ge	Germanium	9/2	7.76	-0.8794677	-19.6	-0.9360306
33	75	As	Arsenic	3/2	100	1.43947	31.4	4.59615
34	77	Se	Selenium	1/2	7.63	0.5350743		5.125388

NMR Properties of Selected Isotopes



Theor. NMR freq. ν_0 calc. from γ and scaled to $^1\text{H} = 100.0$ MHz; Molar Receptivity $R_{\text{M}}(\text{H})$ relative to equal number of protons is proportional to $\gamma^3 / (I+1)$; Receptivity at nat. abundance $R_{\text{NA}}(\text{C})$ relative to ^{13}C ; recommended Reference sample (IUPAC 2001); *experimental* reson. freq. of ref. sample on the unified Ξ scale (at B_0 where TMS (^1H) = 100.0 MHz).

Numbers containing E are in exponential format.

		Theoretical NMR Freq. (free atom)	Molar Receptivity (rel. ^1H)	Receptivity at Nat. Abund. (rel. ^{13}C)	Reference Sample	Measured NMR Freq. (rel. ^1H ref.)
A	Sym	ν_0 [MHz]	$R_{\text{M}}(\text{H})$	$R_{\text{NA}}(\text{C})$	Reference	Ξ [MHz]
1	n	68.4979	3.21E-01			
1	H	100.0000	1.00E+00	5.87E+03	1% Me ₄ Si in CDCl ₃	100.000000
2	D	15.3506	9.65E-03	6.52E-03	(CD ₂) ₂ Si neat	15.350609
3	T	106.6640	1.21E+00		TMS-T ₁	106.663974
3	He	76.1767	4.42E-01	3.48E-03	He gas	76.178976
6	Li	14.7170	8.50E-03	3.79E+00	9.7 m LiCl in D ₂ O	14.716086
7	Li	38.8667	2.94E-01	1.59E+03	9.7 m LiCl in D ₂ O	38.863797
9	Be	14.0536	1.39E-02	8.15E+01	0.43 m BeSO ₄ in D ₂ O	14.051813
10	B	10.7456	1.99E-02	2.32E+01	15% BF ₃ ·Et ₂ O in CDCl ₃	10.743658
11	B	32.0897	1.65E-01	7.77E+02	15% BF ₃ ·Et ₂ O in CDCl ₃	32.083974
13	C	25.1504	1.59E-02	1.00E+00	1% Me ₄ Si in CDCl ₃ DSS in D ₂ O	25.145020 25.144953
14	N	7.2285	1.01E-03	5.90E+00	MeNO ₂ + 10% CDCl ₃	7.226317
15	N	10.1398	1.04E-03	2.23E-02	MeNO ₂ + 10% CDCl ₃ liquid NH ₃	10.136767 10.132767
17	O	13.5617	2.91E-02	6.50E-02	D ₂ O	13.556457
19	F	94.0570	8.32E-01	4.89E+03	CCl ₃ F	94.094011
21	Ne	7.8987	2.46E-03	3.91E-02	Neon gas, 1.1 MPa	7.894296
23	Na	26.4683	9.27E-02	5.45E+02	0.1 M NaCl in D ₂ O	26.451900
25	Mg	6.1260	2.68E-03	1.58E+00	11 M MgCl ₂ in D ₂ O	6.121635
26	Al	10.0399	4.05E-02			
27	Al	26.0774	2.07E-01	1.22E+03	1.1 m Al(NO ₃) ₃ in D ₂ O	26.056859
29	Si	19.8826	7.86E-03	2.16E+00	1% Me ₄ Si in CDCl ₃	19.867187
31	P	40.5178	6.65E-02	3.91E+02	H ₃ PO ₄ external (MeO) ₃ PO internal	40.480742 40.480864
33	S	7.6842	2.27E-03	1.00E-01	(NH ₄) ₂ SO ₄ in D ₂ O (sat.)	7.676000
35	Cl	9.8093	4.72E-03	2.10E+01	0.1 M NaCl in D ₂ O	9.797909
37	Cl	8.1652	2.72E-03	3.88E+00	0.1 M NaCl in D ₂ O	8.155725
39	Ar	8.1228	1.13E-02			
39	K	4.6727	5.10E-04	2.79E+00	0.1 M KCl in D ₂ O	4.666373
40	K	5.8099	5.23E-03	3.59E-03	0.1 M KCl in D ₂ O	5.802018
41	K	2.5648	8.44E-05	3.34E-02	0.1 M KCl in D ₂ O	2.561305
41	Ca	8.1575	1.14E-02			
43	Ca	6.7399	6.43E-03	5.10E-02	0.1 M CaCl ₂ in D ₂ O	6.730029
45	Sc	24.3299	3.02E-01	1.78E+03	0.06 M Sc(NO ₃) ₃ in D ₂ O	24.291747
47	Ti	5.6464	2.10E-03	9.18E-01	TiCl ₄ neat + 10% C ₆ D ₁₂	5.637534
49	Ti	5.6479	3.78E-03	1.20E+00	TiCl ₄ neat + 10% C ₆ D ₁₂	5.639037
50	V	9.9829	5.57E-02	8.18E-01	VOCl ₃ + 5% C ₆ D ₆	9.970309
51	V	26.3362	3.84E-01	2.25E+03	VOCl ₃ + 5% C ₆ D ₆	26.302948
53	Cr	5.6638	9.08E-04	5.07E-01	K ₂ CrO ₄ in D ₂ O (sat.)	5.652496
53	Mn	25.6983	3.56E-01			
55	Mn	24.8400	1.79E-01	1.05E+03	0.82 m KMnO ₄ in D ₂ O	24.789218
57	Fe	3.2448	3.42E-05	4.25E-03	Fe(CO) ₅ + 20% C ₆ D ₆	3.237778
59	Fe	4.0079	3.22E-04			
59	Co	23.6676	2.78E-01	1.64E+03	0.56 m K ₃ [Co(CN) ₆] in D ₂ O	23.727074
60	Co	13.6026	1.01E-01			
61	Ni	8.9517	3.59E-03	2.40E-01	Ni(CO) ₄ + 5% C ₆ D ₆	8.936051
63	Cu	26.5839	9.39E-02	3.82E+02	[Cu(CH ₃ CN) ₄][ClO ₄] in CH ₃ CN (sat.) + 5% C ₆ D ₆	26.515473
65	Cu	28.4250	1.15E-01	2.08E+02	[Cu(CH ₃ CN) ₄][ClO ₄] in CH ₃ CN (sat.) + 5% C ₆ D ₆	28.403693
67	Zn	6.2675	2.87E-03	6.92E-01	Zn(NO ₃) ₂ in D ₂ O (sat.)	6.256803
69	Ga	24.0685	6.97E-02	2.46E+02	1.1 m Ga(NO ₃) ₃ in D ₂ O	24.001354
71	Ga	30.5813	1.43E-01	3.35E+02	1.1 m Ga(NO ₃) ₃ in D ₂ O	30.496704
73	Ge	3.4989	1.41E-03	6.44E-01	Me ₄ Ge + 5% C ₆ D ₆	3.488315
75	As	17.1804	2.54E-02	1.49E+02	0.5 M NaAsF ₆ in CD ₂ CN	17.122614
77	Se	19.1587	7.03E-03	3.15E+00	Me ₂ Se + 5% C ₆ D ₆	19.071513

NMR Properties of Selected Isotopes



Z	A	Sym	Name	I	NA (%)	μ_z / μ_N	Q [fm ²]	γ [10 ⁷ rad s ⁻¹ T ⁻¹]
	79	Se	Selenium (2.95E5 y)	7/2		-1.018	80	-1.393
35	79	Br	Bromine	3/2	50.69	2.106400	30.5	6.725619
	81	Br	Bromine	3/2	49.31	2.270562	25.4	7.249779
36	83	Kr	Krypton	9/2	11.500	-0.970669	25.9	-1.033097
37	85	Rb	Rubidium	5/2	72.17	1.3533515	27.6	2.5927059
	87	Rb	Rubidium (4.81E10 y)	3/2	27.83	2.751818	13.35	8.786403
38	87	Sr	Strontium	9/2	7.00	-1.093603	33.5	-1.163938
39	89	Y	Yttrium	1/2	100	-0.1374154		-1.316279
40	91	Zr	Zirconium	5/2	11.22	-1.30362	-17.6	-2.49743
41	93	Nb	Niobium	9/2	100	6.1705	-32	6.5674
42	95	Mo	Molybdenum	5/2	15.9	-0.9142	-2.2	-1.7514
	97	Mo	Molybdenum	5/2	9.56	-0.9335	25.5	-1.7884
	99	Mo	Molybdenum (65.924 h)	1/2		0.375		3.59
43	99	Tc	Technetium (2.1E5 y)	9/2		5.6847	-12.9	6.0503
44	99	Ru	Ruthenium	5/2	12.76	-0.641	7.9	-1.228
	101	Ru	Ruthenium	5/2	17.06	-0.716	45.7	-1.372
45	103	Rh	Rhodium	1/2	100	-0.08840		-0.84677
46	105	Pd	Palladium	5/2	22.33	-0.642	66	-1.230
47	107	Ag	Silver, Argentum	1/2	51.839	-0.1136797		-1.088918
	109	Ag	Silver	1/2	48.161	-0.13069		-1.2519
48	111	Cd	Cadmium	1/2	12.80	-0.5948861		-5.698315
	113	Cd	Cadmium (7.7E15 y)	1/2	12.22	-0.6223009		-5.960917
49	113	In	Indium	9/2	4.29	5.5289	79.9	5.8845
	115	In	Indium (4.41E14 y)	9/2	95.71	5.5408	81	5.8972
50	115	Sn	Tin	1/2	0.34	-0.91883		-8.8013
	117	Sn	Tin	1/2	7.68	-1.00104		-9.58880
	119	Sn	Tin (Stannum)	1/2	8.59	-1.04728		-10.0317
51	121	Sb	Antimony (Stibium)	5/2	57.21	3.3634	-36	6.4435
	123	Sb	Antimony	7/2	42.79	2.5498	-49	3.4892
	125	Sb	Antimony (2.7586 y)	7/2		2.63		3.60
52	123	Te	Tellurium (9.2E16 y)	1/2	0.89	-0.7369478		-7.059101
	125	Te	Tellurium	1/2	7.07	-0.8885051		-8.510843
53	127	I	Iodine	5/2	100	2.81327	-71	5.38957
	129	I	Iodine (1.57E7 y)	7/2		2.6210	-48	3.5866
54	129	Xe	Xenon	1/2	26.4006	-0.777976		-7.45210
	131	Xe	Xenon	3/2	21.2324	0.691862	-11.4	2.209077
55	133	Cs	C(a)esium	7/2	100	2.582025	-0.343	3.533256
56	135	Ba	Barium	3/2	6.592	0.838627	16.0	2.677690
	137	Ba	Barium	3/2	11.232	0.93734	24.5	2.99287
57	137	La	Lanthanum (6E4 y)	7/2		2.695	26	3.688
57	138	La	Lanthanum (1.05E11 y)	5	0.090	3.713646	45	3.557240
	139	La	Lanthanum	7/2	99.910	2.7830455	20	3.808333
58	139	Ce	Cerium (137.64 d)	3/2		1.06		3.38
	141	Ce	Cerium (32.508 d)	7/2		1.09		1.49
59	141	Pr	Praeseodymium	5/2	100	4.2754	-5.89	8.1907
60	143	Nd	Neodymium	7/2	12.2	-1.065	-63	-1.4574
	145	Nd	Neodymium	7/2	8.3	-0.656	-33	-0.898
61	145	Pm	Promethium (17.7 y)	5/2		3.8	21	7.3
62	147	Sm	Samarium (1.06E11 y)	7/2	14.99	-0.8148	-25.9	-1.115
	149	Sm	Samarium	7/2	13.82	-0.6717	7.5	-0.9192
63	151	Eu	Europium	5/2	47.81	3.4717	90.3	6.6510
	153	Eu	Europium	5/2	52.19	1.5324	241	2.9357
64	155	Gd	Gadolinium	3/2	14.80	-0.2572	127	-0.8212
	157	Gd	Gadolinium	3/2	15.65	-0.3373	135	-1.0770
65	159	Tb	Terbium	3/2	100	2.014	143.2	6.431
66	161	Dy	Dysprosium	5/2	18.889	-0.480	251	-0.920
	163	Dy	Dysprosium	5/2	24.896	0.673	265	1.289
67	163	Ho	Holmium (4570 y)	7/2		4.23	360	5.79
	165	Ho	Holmium	7/2	100	4.132	358	5.654
	166	Ho	Holmium (1200 y)	7		3.60	-340	2.46
68	167	Er	Erbium	7/2	22.869	-0.5639	357	-0.7716
	169	Er	Erbium (9.40 d)	1/2		0.4850		4.646
69	169	Tm	Thulium	1/2	100	-0.231		-2.21
	171	Tm	Thulium (1.92 y)	1/2		-0.228		-2.18
70	171	Yb	Ytterbium	1/2	14.28	0.49367		4.7288
	173	Yb	Ytterbium	5/2	16.13	-0.67989	280	-1.30251
71	175	Lu	Lutetium	7/2	97.41	2.232	349	3.0547

NMR Properties of Selected Isotopes



A	Sym	ν_0 [MHz]	$R_M(H)$	$R_{NA}(C)$	Reference	Ξ [MHz]
79	Se	5.2072	2.97E-03			
79	Br	25.1404	7.94E-02	2.37E+02	0.01 M NaBr in D ₂ O	25.053980
81	Br	27.0997	9.95E-02	2.88E+02	0.01 M NaBr in D ₂ O	27.006518
83	Kr	3.8617	1.90E-03	1.28E+00	Kr gas	3.847600
85	Rb	9.6916	1.06E-02	4.50E+01	0.01 M RbCl in D ₂ O	9.654943
87	Rb	32.8436	1.77E-01	2.90E+02	0.01 M RbCl in D ₂ O	32.720454
87	Sr	4.3508	2.72E-03	1.12E+00	0.5 M SrCl ₂ in D ₂ O	4.333822
89	Y	4.9203	1.19E-04	7.00E-01	Y(NO ₃) ₃ in H ₂ O/D ₂ O	4.900198
91	Zr	9.3354	9.49E-03	6.26E+00	Zr(C ₅ H ₅) ₂ Cl ₂ in CH ₂ Cl ₂ (sat.) + 5% C ₆ D ₆	9.296298
93	Nb	24.5488	4.88E-01	2.87E+03	K[NbCl ₆] in CH ₃ CN / CD ₃ CN (sat.)	24.476170
95	Mo	6.5467	3.27E-03	3.06E+00	2 M Na ₂ MoO ₄ in D ₂ O	6.516926
97	Mo	6.6849	3.49E-03	1.96E+00	2 M Na ₂ MoO ₄ in D ₂ O	6.653695
99	Mo	13.4272	2.42E-03			
99	Tc	22.6161	3.82E-01		NH ₄ TcO ₄ in H ₂ O / D ₂ O	22.508326
99	Ru	4.5903	1.13E-03	8.46E-01	0.3 M K ₄ [Ru(CN) ₆] in D ₂ O	4.605151
101	Ru	5.1274	1.57E-03	1.58E+00	0.3 M K ₄ [Ru(CN) ₆] in D ₂ O	5.161369
103	Rh	3.1652	3.17E-05	1.86E-01	Rh(acac) ₃ in CDCl ₃ (sat.)	3.186447
105	Pd	4.5975	1.13E-03	1.49E+00	K ₂ PdCl ₆ in D ₂ O (sat.)	4.576100
107	Ag	4.0704	6.74E-05	2.05E-01	AgNO ₃ in D ₂ O (sat.)	4.047819
109	Ag	4.6795	1.02E-04	2.90E-01	AgNO ₃ in D ₂ O (sat.)	4.653533
111	Cd	21.3003	9.66E-03	7.27E+00	Me ₂ Cd neat liq.	21.215480
113	Cd	22.2820	1.11E-02	7.94E+00	Me ₂ Cd neat liq.	22.193175
113	In	21.9963	3.51E-01	8.85E+01	0.1 M In(NO ₃) ₃ in D ₂ O + 0.5 M DNO ₃	21.865755
115	In	22.0436	3.53E-01	1.99E+03	0.1 M In(NO ₃) ₃ in D ₂ O + 0.5 M DNO ₃	21.912629
115	Sn	32.8994	3.56E-02	7.11E-01	Me ₄ Sn + 5% C ₆ D ₆	32.718749
117	Sn	35.8430	4.60E-02	2.08E+01	Me ₄ Sn + 5% C ₆ D ₆	35.632259
119	Sn	37.4986	5.27E-02	2.66E+01	Me ₄ Sn + 5% C ₆ D ₆	37.290632
121	Sb	24.0858	1.63E-01	5.48E+02	KSbCl ₆ in CH ₃ CN / CD ₃ CN (sat.)	23.930577
123	Sb	13.0425	4.66E-02	1.17E+02	KSbCl ₆ in CH ₃ CN / CD ₃ CN (sat.)	12.959217
125	Sb	13.4527	5.11E-02			
123	Te	26.3870	1.84E-02	9.61E-01	Me ₂ Te + 5% C ₆ D ₆	26.169742
125	Te	31.8136	3.22E-02	1.34E+01	Me ₂ Te + 5% C ₆ D ₆	31.549769
127	I	20.1462	9.54E-02	5.60E+02	0.01 M KI in D ₂ O	20.007486
129	I	13.4067	5.06E-02			
129	Xe	27.8560	2.16E-02	3.35E+01	XeOF ₄ neat liq.	27.810186
131	Xe	8.2575	2.82E-03	3.51E+00	XeOF ₄ neat liq.	8.243921
133	Cs	13.2073	4.84E-02	2.84E+02	0.1 M CsNO ₃ in D ₂ O	13.116142
135	Ba	10.0092	5.01E-03	1.94E+00	0.5 M BaCl ₂ in D ₂ O	9.934457
137	Ba	11.1874	7.00E-03	4.62E+00	0.5 M BaCl ₂ in D ₂ O	11.112928
137	La	13.7852	5.50E-02			
138	La	13.2970	9.40E-02	4.97E-01	LaCl ₃ in D ₂ O / H ₂ O	13.194300
139	La	14.2356	6.06E-02	3.56E+02	0.01 M LaCl ₃ in D ₂ O	14.125641
139	Ce	12.6514	1.01E-02			
141	Ce	5.5755	3.64E-03			
141	Pr	30.6168	3.35E-01	1.97E+03		
143	Nd	5.4476	3.39E-03	2.43E+00		
145	Nd	3.3555	7.93E-04	3.87E-01		
145	Pm	27.2124	2.35E-01			
147	Sm	4.1678	1.52E-03	1.34E+00		
149	Sm	3.4358	8.52E-04	6.92E-01		
151	Eu	24.8614	1.79E-01	5.04E+02		
153	Eu	10.9737	1.54E-02	4.73E+01		
155	Gd	3.0697	1.45E-04	1.26E-01		
157	Gd	4.0258	3.26E-04	3.00E-01		
159	Tb	24.0376	6.94E-02	4.08E+02		
161	Dy	3.4374	4.74E-04	5.26E-01		
163	Dy	4.8195	1.31E-03	1.91E+00		
163	Ho	21.6369	2.13E-01			
165	Ho	21.1356	1.98E-01	1.16E+03		
166	Ho	9.2072	5.83E-02		(+6 keV excited state)	
167	Er	2.8842	5.04E-04	6.77E-01		
169	Er	17.3658	5.24E-03			
169	Tm	8.2711	5.66E-04	3.32E+00		
171	Tm	8.1637	5.44E-04			
171	Yb	17.6762	5.52E-03	4.63E+00	0.171 M Yb(η-C ₅ Me ₅) ₂ (THF) ₂ in THF	17.499306
173	Yb	4.8688	1.35E-03	1.28E+00		
175	Lu	11.4185	3.13E-02	1.79E+02		

NMR Properties of Selected Isotopes



Z	A	Sym	Name	I	NA (%)	μ_z / μ_N	Q [fm ²]	γ [10 ⁷ rad s ⁻¹ T ⁻¹]
	176	Lu	Lutetium (3.78E10 y)	7	2.59	3.169	497	2.168
72	177	Hf	Hafnium	7/2	18.60	0.7935	337	1.0858
	179	Hf	Hafnium	9/2	13.62	-0.641	379	-0.682
73	179	Ta	Tantalum (1.82 y)	7/2		2.289	337	3.132
	180	Ta	Tantalum (1.2E15 y)	9	0.012	4.825	495	2.568
	181	Ta	Tantalum	7/2	99.988	2.3705	317	3.2438
74	183	W	Tungsten (Wolfram)	1/2	14.31	0.11778476		1.1282407
75	185	Re	Rhenium	5/2	37.40	3.1871	218	6.1057
	187	Re	Rhenium (4.35E10 y)	5/2	62.60	3.2197	207	6.1682
76	187	Os	Osmium	1/2	1.96	0.06465189		0.6192897
	189	Os	Osmium	3/2	16.15	0.659933	85.6	2.107130
77	191	Ir	Iridium	3/2	37.3	0.1507	81.6	0.4812
	193	Ir	Iridium	3/2	62.7	0.1637	75.1	0.5227
78	195	Pt	Platinum	1/2	33.832	0.60952		5.8385
79	197	Au	Gold, Aurum	3/2	100	0.148158	54.7	0.473060
80	199	Hg	Mercury, Hydrargyrum	1/2	16.87	0.5058855		4.845793
	201	Hg	Mercury	3/2	13.18	-0.560226	38.6	-1.788770
81	203	Tl	Thallium	1/2	29.52	1.6222579		15.539339
	205	Tl	Thallium	1/2	70.48	1.6382146		15.692186
82	205	Pb	Lead (1.73E7 y)	5/2		0.7117	23	1.3635
	207	Pb	Lead (Plumbum)	1/2	22.1	0.58219		5.5767
83	209	Bi	Bismuth	9/2	100	4.1103	-51.6	4.3747
84	209	Po	Polonium (102 y)	1/2		0.68		6.51
86	211	Rn	Radon (14.6 h)	1/2		0.601		5.76
87	212	Fr	Francium (19.3 m)	5		4.62	-10	4.43
88	225	Ra	Radium (14.9 d)	1/2		-0.734		-7.03
89	227	Ac	Actinium (21.77 y)	3/2		1.1	170	3.5
90	229	Th	Thorium (7.34E3 y)	5/2		0.46	430	0.88
91	231	Pa	Protactinium (3.25E4 y)	3/2	100	2.01	-172	6.42
92	233	U	Uranium (1.592E5 y)	5/2		0.59	366.3	1.13
	235	U	Uranium (7.04E8 y)	7/2	0.7204	-0.38	493.6	-0.52
	238	U	Uranium (4.468E9 y)	0	99.274		1390	
93	237	Np	Neptunium (2.14E6 y)	5/2		3.14	386.6	6.02
94	239	Pu	Plutonium (2.410E4 y)	1/2		0.203		1.94
	241	Pu	Plutonium (14.4 y)	5/2		-0.68	560	-1.30
95	241	Am	Americium (432.7 y)	5/2		1.58	314	3.03
	243	Am	Americium (7.37E3 y)	5/2		1.50	286	2.87
96	243	Cm	Curium (29.1 y)	5/2		0.41		0.79
	245	Cm	Curium (8.48E3 y)	7/2		0.5		0.68
	247	Cm	Curium (1.56E7 y)	9/2		0.37		0.39
97	247	Bk	Berkelium (1.4E2 y)	(3/2)		no data		
	249	Bk	Berkelium (320 d)	7/2		2.0		2.7
98	251	Cf	Californium (9.0E2 y)	1/2		no data		
99	252	Es	Einsteinium (472 d)	(5)		no data		
	253	Es	Einsteinium (20.47 d)	7/2		4.10	670	5.61
100	253	Fm	Fermium (3.0 d)	(1/2)		no data		
	257	Fm	Fermium (100.5 d)	(9/2)		no data		

This Table (updated Oct. 2009) was assembled and calculated by W.E. Hull using information from the following sources:

- De Laeter et al. *Pure Appl Chem* 75 (2003) 683-800. (isotope abundances)
- Harris RK, et al. *Pure Appl Chem* 73 (2001) 1795-1818 and 80 (2008) 59-84. (shift references)
- Mills I, et al. *Quantities, Units and Symbols in Physical Chemistry* (IUPAC recommendations 1993, corrections 1995). Blackwell Scientific (1993, 1995).
- Pyykkö P. Spectroscopic nuclear quadrupole moments. *Mol. Phys.* 99 (2001) 1617-1629.

NMR Properties of Selected Isotopes



A	Sym	ν_0 [MHz]	$R_M(H)$	$R_M(C)$	Reference	Δ [MHz]
176	Lu	8.1049	3.98E-02	6.05E+00		
177	Hf	4.0588	1.40E-03	1.53E+00		
179	Hf	2.5502	5.47E-04	4.38E-01		
179	Ta	11.7085	3.37E-02			
180	Ta	9.5979	1.06E-01	7.48E-02	(+77 keV excited state)	
181	Ta	12.1254	3.74E-02	2.20E+02	KTaCl ₆ in CH ₃ CN (sat.)	11.989600
183	W	4.2174	7.50E-05	6.31E-02	1 M Na ₂ WO ₄ in D ₂ O	4.166387
185	Re	22.8233	1.39E-01	3.05E+02	0.1 M KReO ₄ in D ₂ O	22.524600
187	Re	23.0568	1.43E-01	5.26E+02	0.1 M KReO ₄ in D ₂ O	22.751600
187	Os	2.3149	1.24E-05	1.43E-03	0.98 M OsO ₄ in CCl ₄	2.282331
189	Os	7.8765	2.44E-03	2.32E+00	0.98 M OsO ₄ in CCl ₄	7.765400
191	Ir	1.7986	2.91E-05	6.38E-02		
193	Ir	1.9538	3.73E-05	1.37E-01		
195	Pt	21.8243	1.04E-02	2.07E+01	1.2 M Na ₂ PtCl ₆ in D ₂ O	21.496784
197	Au	1.7683	2.76E-05	1.62E-01		
199	Hg	18.1136	5.94E-03	5.89E+00	Me ₂ Hg neat liq. (toxic!)	17.910822
201	Hg	6.6864	1.49E-03	1.16E+00	Me ₂ Hg neat liq. (toxic!)	6.611583
203	Tl	58.0862	1.96E-01	3.40E+02	Tl(NO ₃) ₃	57.123200
205	Tl	58.6575	2.02E-01	8.36E+02	Tl(NO ₃) ₃	57.683838
205	Pb	5.0966	1.54E-03			
207	Pb	20.8458	9.06E-03	1.18E+01	Me ₂ Pb + 5% C ₆ D ₆	20.920599
209	Bi	16.3525	1.44E-01	8.48E+02	Bi(NO ₃) ₃ sat. in conc. HNO ₃ + 50% D ₂ O	16.069288
209	Po	24.3479	1.44E-02			
211	Rn	21.5193	9.97E-03			
212	Fr	16.5423	1.81E-01			
225	Ra	26.2814	1.82E-02			
227	Ac	13.1288	1.13E-02			
229	Th	3.2941	4.17E-04			
231	Pa	23.9899	6.90E-02	4.06E+02		
233	U	4.2251	8.80E-04			
235	U	1.9437	1.54E-04	6.53E-03	UF ₆ + 10% C ₆ D ₆	1.841400
238	U					
237	Np	22.4860	1.33E-01			
239	Pu	7.2686	3.84E-04			
241	Pu	4.8696	1.35E-03			
241	Am	11.3146	1.69E-02			
243	Am	10.7417	1.45E-02			
243	Cm	2.9361	2.95E-04			
245	Cm	2.5576	3.51E-04			
247	Cm	1.4720	1.05E-04			
249	Bk	10.2302	2.25E-02			
253	Es	20.9719	1.94E-01			

Stone NJ. *Table of Nuclear Magnetic Dipole and Electric Quadrupole Moments (2001)*

[http://www.nndc.bnl.gov/nndc/stone_moments/nuclear-moments.pdf].

LBNL Isotopes Project Nuclear Data Dissemination Home Page. *Table of Nuclear Moments*

[<http://ie.lbl.gov/toipdf/mometbl.pdf>].

NUDAT 2 half-life data: <http://www.nndc.bnl.gov/>

Isotopes sorted according to spin and nucleon numbers

Isotope			Spin	Isotope			Spin	Isotope			Spin
1	H	Hydrogen	1/2	39	K	Potassium	3/2	173	Yb	Ytterbium	5/2
3	H	Tritium *	1/2	41	K	Potassium	3/2	185	Re	Rhenium	5/2
3	He	Helium	1/2	53	Cr	Chromium	3/2	187	Re	Rhenium	5/2
13	C	Carbon	1/2	61	Ni	Nickel	3/2	229	Th	Thorium *	5/2
15	N	Nitrogen	1/2	63	Cu	Copper	3/2	237	Np	Neptunium *	5/2
19	F	Fluorine	1/2	65	Cu	Copper	3/2	241	Am	Americium *	5/2
29	Si	Silicon	1/2	69	Ga	Gallium	3/2	243	Am	Americium *	5/2
31	P	Phosphorus	1/2	71	Ga	Gallium	3/2	10	B	Boron	3
57	Fe	Iron	1/2	75	As	Arsenic	3/2	39	Ar	Argon *	7/2
77	Se	Selenium	1/2	79	Br	Bromine	3/2	43	Ca	Calcium	7/2
89	Y	Yttrium	1/2	81	Br	Bromine	3/2	45	Sc	Scandium	7/2
103	Rh	Rhodium	1/2	87	Rb	Rubidium	3/2	49	Ti	Titanium	7/2
107	Ag	Silver	1/2	131	Xe	Xenon	3/2	51	V	Vanadium	7/2
109	Ag	Silver	1/2	135	Ba	Barium	3/2	59	Co	Cobalt	7/2
111	Cd	Cadmium	1/2	137	Ba	Barium	3/2	123	Sb	Antimony	7/2
113	Cd	Cadmium	1/2	139	Ce	Cerium *	3/2	133	Cs	C(a)esium	7/2
115	Sn	Tin	1/2	155	Gd	Gadolinium	3/2	139	La	Lanthanum	7/2
117	Sn	Tin	1/2	157	Gd	Gadolinium	3/2	143	Nd	Neodymium	7/2
119	Sn	Tin	1/2	159	Tb	Terbium	3/2	145	Nd	Neodymium	7/2
123	Te	Tellurium	1/2	189	Os	Osmium	3/2	147	Sm	Samarium	7/2
125	Te	Tellurium	1/2	191	Ir	Iridium	3/2	149	Sm	Samarium	7/2
129	Xe	Xenon	1/2	193	Ir	Iridium	3/2	165	Ho	Holmium	7/2
169	Tm	Thulium	1/2	197	Au	Gold	3/2	167	Er	Erbium	7/2
171	Yb	Ytterbium	1/2	201	Hg	Mercury	3/2	175	Lu	Lutetium	7/2
183	W	Tungsten	1/2	227	Ac	Actinium *	3/2	177	Hf	Hafnium	7/2
187	Os	Osmium	1/2	231	Pa	Protactinium *	3/2	181	Ta	Tantalum	7/2
195	Pt	Platinum	1/2	17	O	Oxygen	5/2	235	U	Uranium *	7/2
199	Hg	Mercury	1/2	25	Mg	Magnesium	5/2	245	Cm	Curium *	7/2
203	Tl	Thallium	1/2	27	Al	Alumin(i)um	5/2	249	Bk	Berkelium *	7/2
205	Tl	Thallium	1/2	47	Ti	Titanium	5/2	253	Es	Einsteinium *	7/2
207	Pb	Lead	1/2	55	Mn	Manganes	5/2	73	Ge	Germanium	9/2
209	Po	Polonium *	1/2	67	Zn	Zinc	5/2	83	Kr	Krypton	9/2
211	Rn	Radon *	1/2	85	Rb	Rubidium	5/2	87	Sr	Strontium	9/2
225	Ra	Radium *	1/2	91	Zr	Zirconium	5/2	93	Nb	Niobium	9/2
239	Pu	Plutonium *	1/2	95	Mo	Molybdenum	5/2	99	Tc	Technetium *	9/2
251	Cf	Californium *	1/2	97	Mo	Molybdenum	5/2	113	In	Indium	9/2
2	H	Deuterium	1	99	Ru	Ruthenium	5/2	115	In	Indium	9/2
6	Li	Lithium	1	101	Ru	Ruthenium	5/2	179	Hf	Hafnium	9/2
14	N	Nitrogen	1	105	Pd	Palladium	5/2	209	Bi	Bismuth	9/2
7	Li	Lithium	3/2	121	Sb	Antimony	5/2	138	La	Lanthanum	5
9	Be	Beryllium	3/2	127	I	Iodine	5/2	212	Fr	Francium *	5
11	B	Boron	3/2	141	Pr	Praeseodymium	5/2	50	V	Vanadium	6
21	Ne	Neon	3/2	145	Pm	Promethium *	5/2	176	Lu	Lutetium	7
23	Na	Sodium	3/2	151	Eu	Europium	5/2				
33	S	Sulfur	3/2	153	Eu	Europium	5/2				
35	Cl	Chlorine	3/2	161	Dy	Dysprosium	5/2				
37	Cl	Chlorine	3/2	163	Dy	Dysprosium	5/2				

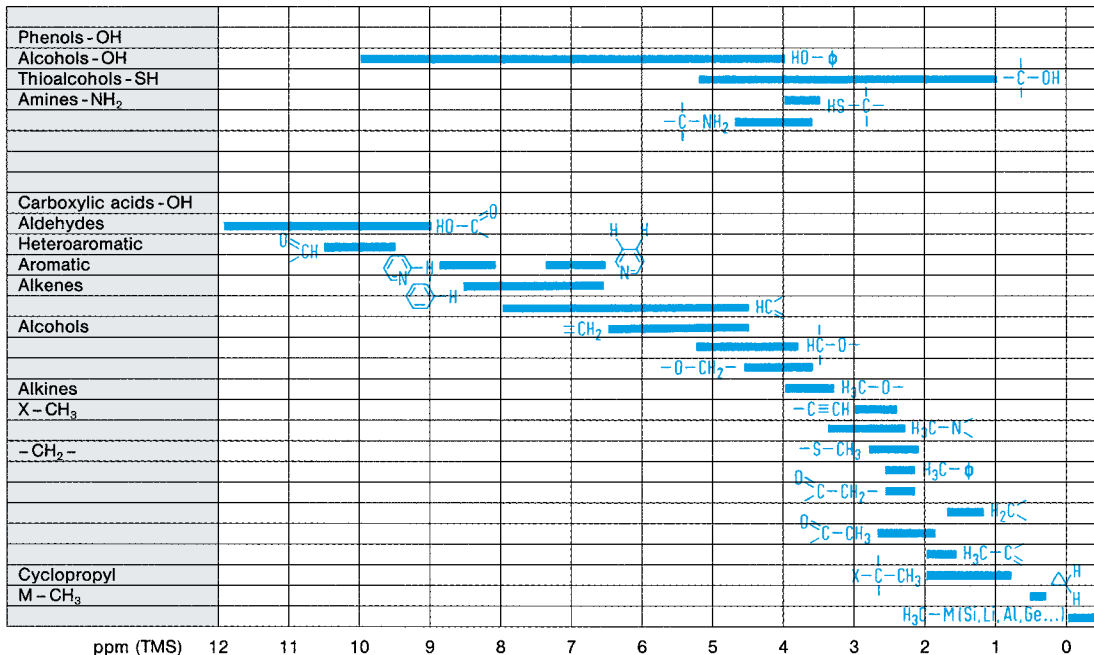
* Unstable isotope with lifetime suitable for NMR.

Properties of Selected Deuterated Solvents for NMR

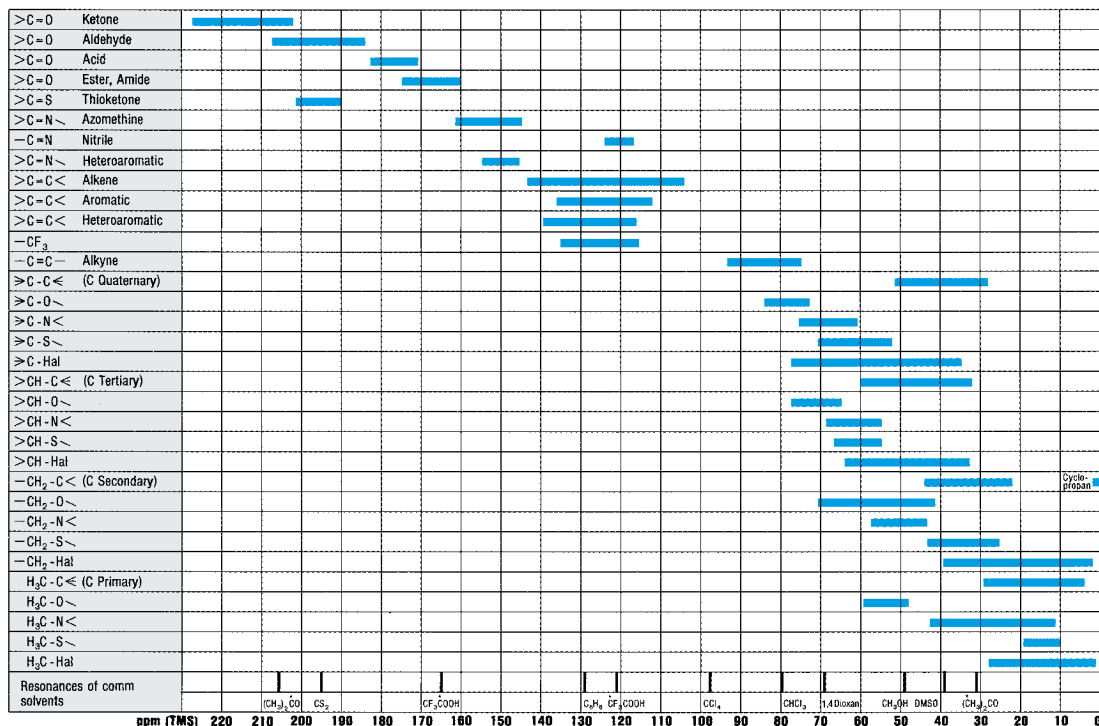
Solvent	Formula	MW _{ave}	Density	MP	BP	RI	Dielec.	¹ H shift (Mult.)	J(HD)	¹³ C Shift (Mult.)	J(CD)	H ₂ O/HDO Shift [ppm]
			[d ₄ ²⁰]	[°C]	[°C]	[n _D ²⁰]	[ε]	[ppm]	[Hz]	[ppm]	[Hz]	
Acetic Acid-d4	C ₂ D ₄ O ₂	64.08	1.119	15.9	115.5	1.368	6.1	11.65 2.04 (5)	2.2	178.99 20 (7)	20	11.5
Acetone-d6	C ₃ D ₆ O	64.12	0.872	-93.8	55.5	1.3554	20.7	2.05 (5)	2.2	29.92 (7) 206.68 (13)	19.4 0.9	2.84/ 2.81
Acetonitrile-d3	C ₂ D ₃ N	44.07	0.844	-46	80.7	1.3406	37.5	1.94 (5)	2.5	1.39 (7) 118.69	21	2.12
Benzene-d6	C ₆ D ₆	84.15	0.950	6.8	79.1	1.4986	2.3	7.16		128.39 (3)	24.3	0.4
Chloroform-d1	CDCl ₃	120.38	1.500	-64.1	60.9	1.4445	4.8	7.24		77.23 (3)	32	1.55
Cyclohexane-d12	C ₆ D ₁₂ O	96.24	0.890	7	78		2	1.38		26.43 (5)	19	0.80
Deuterium oxide	D ₂ O	20.03	1.107	3.8	101.4	1.328	78.5	4.81				
1,2-Dichloroethane-d4	C ₂ D ₄ Cl ₂	102.99	1.307	-35	83	1.443		3.72 (5)		43.6 (5)	23.5	
Dichloromethane-d2	CD ₂ Cl ₂	86.95	1.362	-97	39.5	1.362		5.32 (3)	1.1	54 (5)	27.2	1.52
Diethylether-d10	C ₄ D ₁₀ O	84.19	0.78	-116.3	34.6			3.34 (m) 1.07 (m)		65.3 (5) 14.5 (7)	21 19	
Diethylene glycol dimethyl ether-d14 (diglyme-d14)	C ₆ D ₁₄ O ₃	148.26	0.95	-68	162			3.49 (br) 3.40 (br) 3.22 (5)	1.5	70.7 (5) 70 (5) 57.7 (7)	21 21 21	
1,2-Dimethoxyethane-d10 (glyme-d10)	C ₄ D ₁₀ O ₂	100.18	0.86	-58	83			3.40 (m) 3.22 (5)	1.6	71.7 (5) 57.8 (7)	21 21	
N,N-Dimethyl-formamide-d7	C ₃ D ₇ NO	80.14	1.04	-60	153	1.428	36.7	8.03 2.92 (5) 2.75 (5)	1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.45
Dimethyl sulfoxide-d6	C ₂ D ₆ O _S	84.17	1.190	20.2	190	1.4758	46.7	2.50 (5)	1.9	39.51 (7)	21.0	3.3
1,4-Dioxane-d6	C ₄ D ₈ O ₂	96.16	1.129	12	99	1.4198	2.2	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d6	C ₂ D ₆ O	52.11	0.888	-114.5	78	1.358	24.5	5.29 3.56 1.11 (m)		56.96 (5) 1731 (7)	22 19	5.2
Methanol-d4	CD ₃ O	36.07	0.89	-99	65	1.3256	32.7	4.87 3.31 (5)	1.7	49.15 (7)	21.4	4.86
Methyl cyclohexane-d14	C ₇ D ₁₄	112.27	0.77	-126	101	1.4189						
Nitrobenzene-d5	C ₆ D ₅ NO ₂	128.14	1.253	6	211	1.5498		8.11 (br) 7.67 (br) 7.50 (br)		148.6 134.8 (3) 129.5 (3) 123.5 (3)	24.5 25 26	2.42
Nitromethane-d3	CD ₃ NO ₂	64.06	1.19	-26	100	1.3795		4.33 (5)		62.8 (7)	22	2.2
2-Propanol-d8	C ₃ D ₈ O	68.15	0.786	-89.5	82.4	1.3728		5.12 3.89 (br) 1.10 (br)		62.9 (3) 24.2 (7)	21.5 19	
Pyridine-d5	C ₅ D ₅ N	84.13	1.02	-41	114	1.5079	12.4	8.74 7.58 7.22		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	4.97
Tetrachloroethane-d2	C ₂ D ₂ Cl ₄	169.86	1.7	-43	146	1.493		5.91 (5)		74.2 (5)		1.5
Tetrahydrofuran-d8	C ₄ D ₈ O	80.16	0.99	-108	64	1.4035	7.6	3.58 1.73		67.57 (5) 25.37 (5)	22.2 20.2	2.42
Toluene-d8	C ₇ D ₈	100.19	0.94	-85	109	1.4932	2.4	7.09 (m) 7.00 6.98 (m) 2.09 (5)	2.3	137.86 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	23 24 24 19	0.45
2,2,2-Trifluoroacetic Acid-d1	C ₂ DF ₃ O ₂	115.03	1.50	-15	71	1.30		11.50		164.2 (4) 116.6 (4)		11.5
2,2,2-Trifluoroethanol-d3	C ₂ D ₃ F ₃	87.06	1.42	-44	77	1.30		5.02 3.88 (4x3)	2 (9)	126.3 (4) 61.5 (4x5)	22	5

This Table summarizes the physical properties of deuterated solvents and the chem. shifts (rel. to TMS) and deuterium couplings for the solvent signals and the approximate shifts for residual water (last column).

¹H Chemical Shifts in Organic Compounds

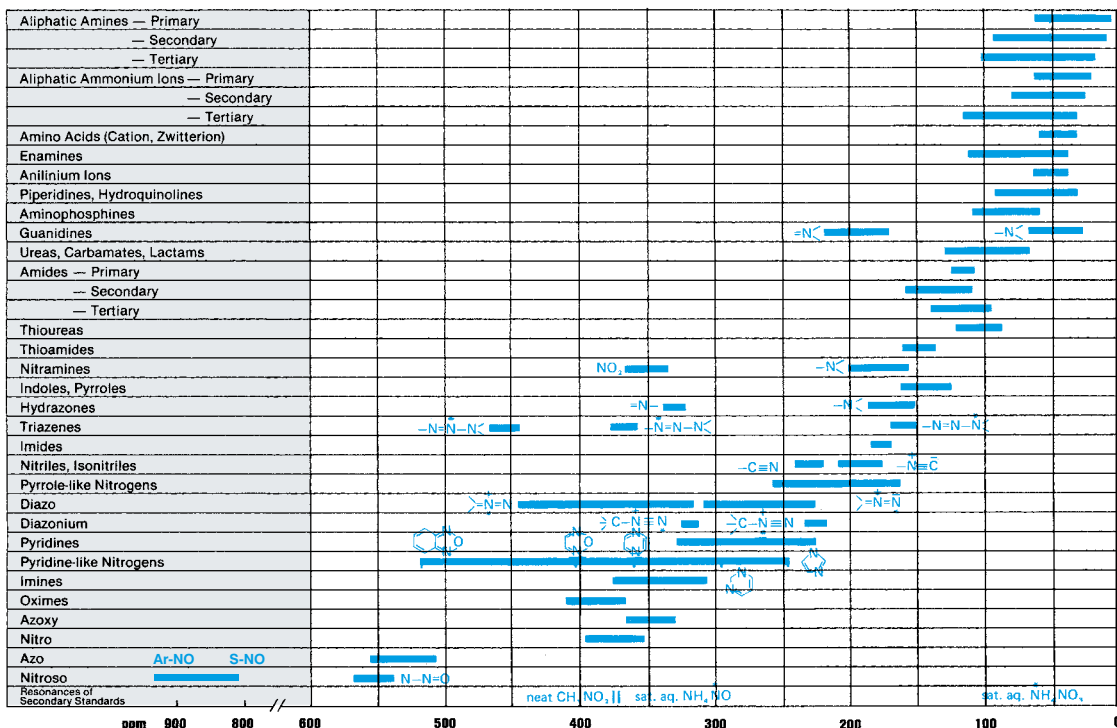


¹³C Chemical Shifts in Organic Compounds*



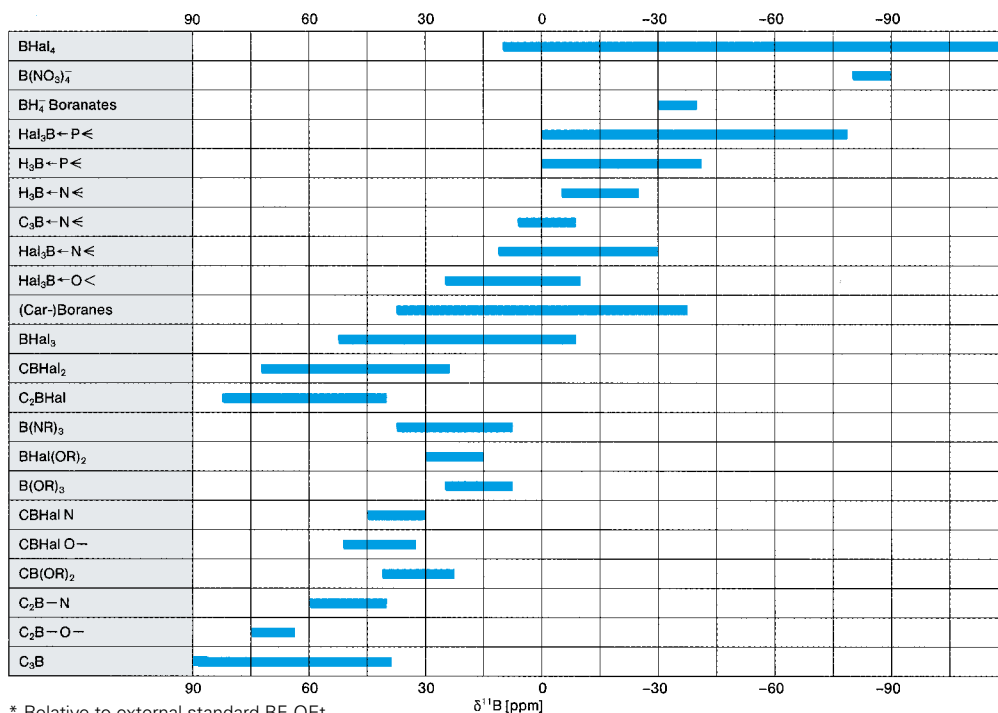
* Relative to internal tetramethylsilane.

¹⁵N Chemical Shifts in Organic Compounds*



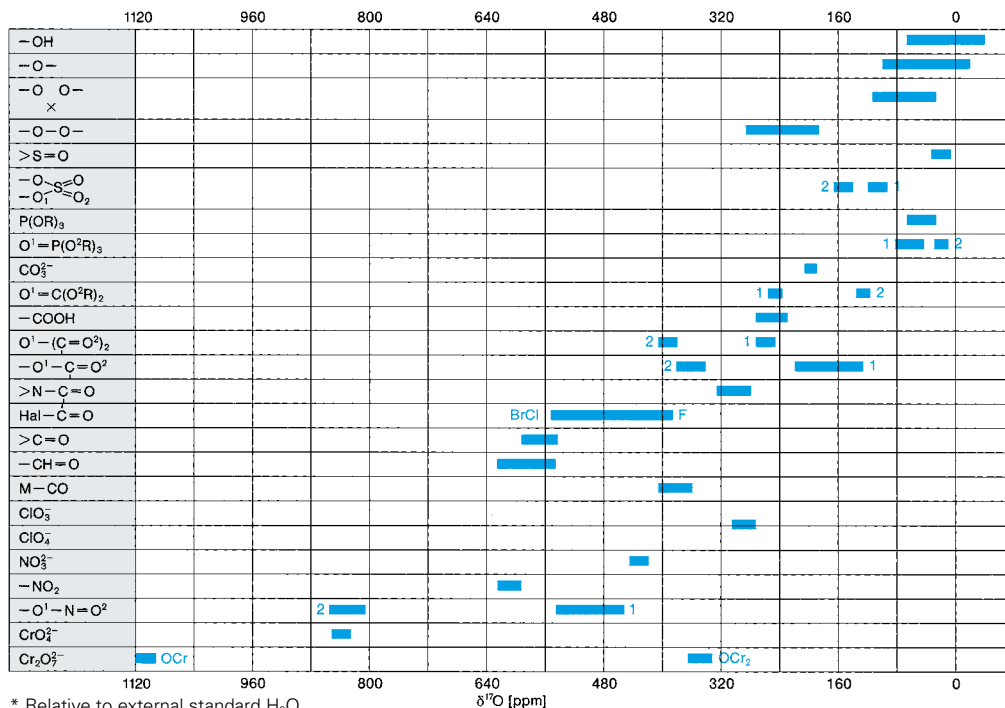
* Relative to external liquid ammonia at 25°C. Data taken from: G. C. Levy and R. L. Lichter: "Nitrogen-15 Nuclear Magnetic Resonance Spectroscopy", J. Wiley, 1979.

¹¹B Chemical Shifts*

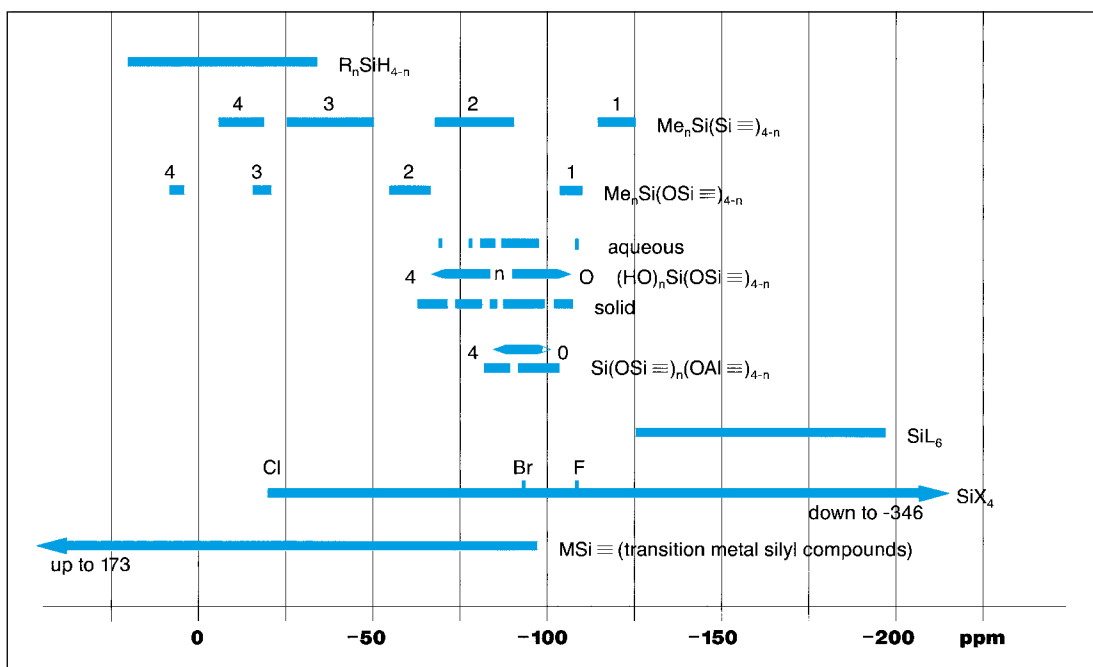


* Relative to external standard BF₃OEt₂

¹⁷O Chemical Shifts*

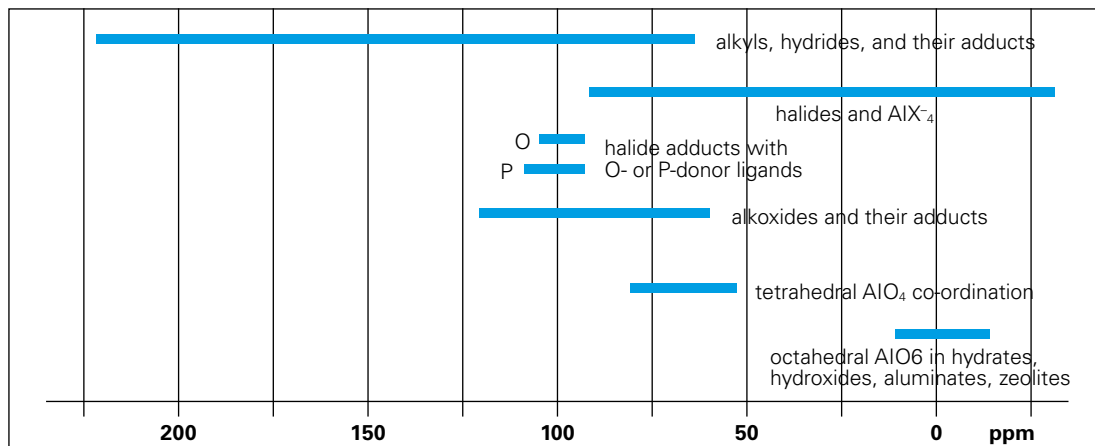


²⁹Si Chemical Shifts*



* Relative to Si(CH₃)₄.

²⁷Al Chemical Shifts*



* Relative to $\text{Al}(\text{H}_2\text{O})_6^{3+}$.

MRI Tables

Abbreviations and Acronyms Used in Magnetic Resonance Imaging

Method	Description	Equivalent acronyms
SINGLEPULSE	Basic pulse-and-acquire spectroscopy	FID
NSPECT	Non-localized spectroscopy with NOE and decoupling options	FID
CSI	Chemical shift imaging with optional PRESS localization	
PRESS	Localized MRS with double spin echo	
STEAM	Localized MRS with stimulated echo (for short TE)	
ISIS	Localized MRS with inversion-based voxel definition	OSIRIS
DtiEpi	Diffusion tensor imaging with EPI (SE and STE)	PGSE-EPI
DtiStandard	Diffusion tensor imaging with 2DFT (SE and STE)	PGSE
EPI	Echo-Planar Imaging (GE and SE), single-shot or interleaved, with navigator-based phase stabilization and automatic ghost correction	
FAIR_EPI	Pulsed arterial spin labelling-based perfusion imaging with EPI	
FC2D_ANGIO	Time-of-flight angiography flow-compensated	TOFangio
FL2D_ANGIO	Time-of-flight angiography w/o flow-comp. (short TE)	
FISP	Fast gradient echo with steady state signal selection (FID, echo or fully balanced), and optional inversion recovery for T1 mapping.	FLASH, FAST, FISP, PSIF, CE-FAST, SSFP, GRASS, TrueFISP
FLASH	Gradient echo	FISP, GRASS, FAST
GEFC	Gradient echo with flow compensation	
MDEFT	T1-weighted hi-res imaging with inversion-recovery preparation	MPRAGE
MGE	Multiple gradient echo	
MSME	Multiple spin echo including T2 mapping	
RARE	Fast spin echo based on CPMG sequence	FSE, TSE
RAREVTR	RARE with variable TR for simultaneous T1&T2 mapping	
RAREst	Fast spin echo for short TE using slew-rate-optimized gradients	HASTE
FLOW_MAP	Quantitative flow mapping and PC-angio	
UTE	Ultra-short TE radial scan	
FieldMap	Quantitative B0 mapping, part of the MAPSHIM tool for localized high-order shimming	
SPIRAL	Fast MRI with spiral k-space scan	
IntraGate-FLASH	Cardiac and respiration-cine with retrospective (trigger-free) gating	

Additivity Parameters for ^{13}C Chemical Shifts in Substituted Benzenes

$\delta_i = 128.5 + S_i(\delta_i)$, $S_i(\delta_i)$ refers to the carbon atom bearing the substituent

Substituent	$S_i(\delta_i)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$	Substituent	$S_i(\delta_i)$	$S_i(\delta_o)$	$S_i(\delta_m)$	$S_i(\delta_p)$
-H	0.0	0.0	0.0	0.0	-I	-32.3	9.9	2.6	-0.4
-CH ₃	9.3	0.6	0.0	-3.1	-OH	26.9	-12.7	1.4	-7.3
-CH ₂ CH ₃	15.7	-0.6	-0.1	-2.8	-OCH ₃	30.2	-14.7	0.9	-8.1
-CH(CH ₃) ₂	20.1	-2.0	0.0	-2.5	-NH ₂	19.2	-12.4	1.3	-9.5
-C(CH ₃) ₃	22.1	-3.4	-0.4	-3.1	-N(CH ₃) ₂	22.4	-15.7	0.8	-11.8
-Cyclopropyl	15.1	-3.3	-0.6	-3.6	-N(C ₆ H ₅) ₂	19.3	-4.4	0.6	-5.9
-CH ₂ Cl	9.1	0.0	0.2	-0.2	-NO ₂	19.6	-5.3	0.8	6.0
-CH ₂ Br	9.2	0.1	0.4	-0.3	-CN	-16.0	3.5	0.7	4.3
-CF ₃	2.6	-2.2	0.3	3.2	-NCO	5.7	-3.6	1.2	-2.8
-CH ₂ OH	13.0	-1.4	0.0	-1.2	-SC(CH ₃) ₃	4.5	9.0	-0.3	0.0
-CH=CH ₂	7.6	-1.8	-1.8	-3.5	-COH	9.0	1.2	1.2	6.0
-C≡CH	-6.1	3.8	0.4	-0.2	-COCH ₃	9.3	0.2	0.2	4.2
-C ₆ H ₅	13.0	-1.1	0.5	-1.0	-COOH	2.4	1.6	-0.1	4.8
-F	35.1	-14.3	0.9	-4.4	-COO ⁻	7.6	0.8	0.0	2.8
-Cl	6.4	0.2	1.0	-2.0	-COOCH ₃	2.1	1.2	0.0	4.4
-Br	-5.4	3.3	2.2	-1.0	-COCl	4.6	2.9	0.6	7.0

Some Representative ^{19}F Chemical Shifts Referenced to CFCl_3

	δ / ppm		δ / ppm		δ / ppm
MeF	-271.9	CFBr ₃	7.4	FCH=CH ₂	-114
EtF	-213	CF ₂ Br ₂	7	F ₂ C=CH ₂	-81.3
CF ₂ H ₂	-1436	CFH ₂ Ph	-207	F ₂ C=CF ₂	-135
CF ₃ R	-60 to -70	CF ₂ Cl ₂	-8	C ₆ F ₆	-163
AsF ₅	-66	[AsF ₆] ⁻	-69.5	[BeF ₄] ⁻	-163
BF ₃	-131	ClF ₃	116; -4	ClF ₅	247; 412
IF ₇	170	MoF ₆	-278	ReF ₇	345
SeF ₆	55	[SbF ₆] ⁻	-109	SbF ₅	-108
[SiF ₆] ²⁻	-127	TeF ₆	-57	WF ₆	166
XeF ₂	258	XeF ₄	438	XeF ₆	550

Some Representative ^{31}P Chemical Shifts Referenced to 85 % H_3PO_4

(a) Phosphorus (III) compounds			
	δ / ppm		δ / ppm
PMe ₃	-62	PMeF ₂	245
PEt ₃	-20	PMeH ₂	-163.5
P(<i>n</i> -Pr) ₃	-33	PMeCl ₂	192
P(<i>i</i> -Pr) ₃	-19.4	PMeBr ₂	184
P(<i>n</i> -Bu) ₃	-32.5	PMe ₂ F	186
P(<i>i</i> -Bu) ₃	-45.3	PMe ₂ H	-99
P(<i>s</i> -Bu) ₃	7.9	PMe ₂ Cl	96.5
P(<i>t</i> -Bu) ₃	63	PMe ₂ Br	90.5

(b) Phosphorus (V) compounds			
	δ / ppm		δ / ppm
Me ₃ PO	36.2	Me ₃ PS	59.1
Et ₃ PO	48.3	Et ₃ PS	54.5
[ME ₄ P] ⁺	24.4	[Et ₄ P] ⁺	40.1
[PO ₄] ³⁻	6.0	[PS ₄] ³⁻	87
PF ₅	-80.3	[PF ₆] ⁻	-145
PCl ₅	-80	[PCl ₄] ⁺	86
MePF ₄	-29.9	[PCl ₆] ⁻	-295
Me ₃ PF ₂	-158	Me ₂ PF ₃	8.0

Some Important Silylated Compounds Used as ¹H Shift References

Name	Chemical formula	Abbreviation	Molecular weight	Boiling or melting point (°C)	δ ¹ H ppm rel. TMS
Tetramethylsilane	(CH ₃) ₄ Si	TMS	88.2	BP = 26.3	0
Hexamethyldisilane	(CH ₃) ₃ Si-Si(CH ₃) ₃	HMDS	146.4	BP = 112.3	0.037
Hexamethyldisiloxane	(CH ₃) ₃ Si-O-Si(CH ₃) ₃	HMDSO	162.4	BP = 100	0.055
Hexamethyldisilazane	(CH ₃) ₃ Si-NH-Si(CH ₃) ₃	HMDSA	161.4	BP = 125	0.042
3-(trimethylsilyl)propane sulfonic acid sodium salt 4,4-dimethyl-4-silapentane sodium sulfonate	(CH ₃) ₃ Si(CH ₂) ₃ SO ₃ Na	TSPSA DSS	218.3	MP = 200	0.015
3-(trimethylsilyl)propionic acid sodium salt 4,4-dimethyl-4-silapentane sodium carboxylate	(CH ₃) ₃ Si(CH ₂) ₂ COONa	TSP DSC	168.2	MP > 300	0.000
3-(trimethylsilyl) 2,2,3,3-tetra-deuteriopropionic acid sodium salt	(CH ₃) ₃ Si(CD ₂) ₂ COONa	TSP-d ₄	172.2	MP > 300	0.000
Octamethylcyclotetrasiloxane	(CH ₃) ₂ Si[O-Si(CH ₃) ₂] ₃ -O	OCTS	296.8	BP = 175 MP = 16.8	0.085
1,1,3,3,5,5-hexakis-(trideuteromethyl)-1,3,5-trisilacyclohexane	(CD ₃) ₂ Si-CH ₂ -Si(CD ₃) ₂ CH ₂ -Si(CD ₃) ₂ -CH ₂	CS-d ₁₈	216.6	BP = 208	-0.327
Tetrakis-(trimethylsilyl)-methane	[(CH ₃) ₃ Si] ₄ C	TTSM	304.8	MP = 307	0.236

Enhancement Factors η_{NOE} and η_{INEPT} for X {¹H} Nuclear Overhauser and INEPT Experiments

X	¹⁹ F	³¹ P	¹¹ B	¹³ C	¹⁵ N	²⁹ Si	⁵⁷ Fe	¹⁰³ Rh	¹⁰⁹ Ag	¹¹⁹ Sn	¹⁸³ W
η_{NOE}^a	0.53	1.24	1.56	1.99	-4.93	-2.52	15.41	-15.80	-10.68	-1.33	11.86
η_{INEPT}^b	1.06	2.47	3.12	3.98	-9.86	-5.03	30.82	-31.59	-21.37	-2.67	23.71

^a The maximum possible intensity enhancement is equal to 1 + η_{NOE} in the extreme narrowing limit.

^b For ¹⁹F or ³¹P as polarization source (irradiated nucleus) the factors η_{NOE} and η_{INEPT} are reduced by the factor 0.941 [$\gamma(^{19}\text{F})/\gamma(^1\text{H})$] and 0.405 [$\gamma(^{31}\text{P})/\gamma(^1\text{H})$]

Relevant Properties of Cryogenic Fluids

(Liquid helium and nitrogen are used in supercon magnets)

Cryogen	Normal Boiling Point (K)	Latent Heat (J/g)	Amount of Liquid Evaporated by 1 Watt (l/hour)	Liquid Density (g/ml)	Gas Density at NTP (g/ml)	Liquid to NTP Gas Volume Ratio	Enthalpy Change (gas) B.P. to 77 K (J/mole)	Enthalpy Change (gas) 77 to 300 K (J/mole)
Liquid Helium	4.2	20.9	1.038	0.125	1.79 × 10 ⁻⁴	1 : 700	384	1157
Liquid Hydrogen	20.39	443	0.115	0.071	8.99 × 10 ⁻⁵	1 : 790	590	2900
Liquid Nitrogen	77.55	198	0.023	0.808	1.25 × 10 ⁻³	1 : 650	-	234
Liquid Oxygen	90.19	212.5	0.015	1.014	1.43 × 10 ⁻³	1 : 797	-	From BP: 193

NTP = normal room temperature and atmospheric pressure

¹H, ¹H Coupling Constants in Selected Organic Molecules

	X	³ J _{cis}	³ J _{trans}	² J	H ₃ C-CH ₂ -X	X	³ J
	H	11.6	19.1	2.5			Li
Li	19.3	23.9	7.1		Si(C ₂ H ₅) ₃	8.0	
COOH	10.2	17.2	1.7		H	7.5	
CN	11.75	17.92	0.91		C ₆ H ₅	7.62	
C ₆ H ₅	11.48	18.59	1.08		CN	7.60	
CH ₃	10.02	16.81	2.08		I	7.45	
OCH ₃	7.0	14.1	-2.0		Br	7.33	
Cl	1.3	14.6	-1.4		CH ₃	7.26	
Br	7.1	15.2	-1.8		Cl	7.23	
F	4.65	12.75	-3.2		N(C ₂ H ₅) ₂	7.13	
					OC ₂ H ₅	6.97	
					⁺ O(C ₂ H ₅) ₂	4.7	

	X	³ J(1,2)	³ J(1,3)	³ J(2,4)	³ J(3,5)	³ J(2,5)	² J(2,3)
	H	8.97	5.58	8.97	8.97	5.58	-4.34
Cl	7.01	3.58	10.26	10.58	7.14	-6.01	
Br	7.13	3.80	10.16	10.45	7.01	-6.12	
I	7.51	4.37	9.89	9.97	6.63	-5.94	
NH ₂	6.63	3.55	9.65	9.89	6.18	-4.29	
CN	8.43	5.12	9.18	9.49	7.08	-4.72	
COOH	8.04	4.57	9.26	9.66	7.14	-4.00	
COCl	7.88	4.43	9.19	9.99	7.59	-4.46	
COCH ₃	7.96	4.55	8.76	9.60	6.94	-3.41	

	X	³ J(1,2)	⁴ J(1,3)	⁵ J(1,4)	⁴ J(1,5)	³ J(2,3)	⁴ J(2,4)
	H	7.54	1.37	0.66	1.37	7.54	1.37
Li	6.73	1.54	0.77	0.74	1.42	1.29	
CH ₃	7.64	1.25	0.60	1.87	7.52	1.51 ^a	
COOCH ₃	7.86	1.35	0.63	1.79	7.49	1.31	
I	7.93	1.14	0.47	1.88	7.47	1.75	
Br	8.05	1.12	0.46	2.1	7.44	1.78	
Cl	8.05	1.13	0.48	2.27	7.51	1.72	
NH ₂	8.02	1.11	0.47	2.53	7.39	1.60	
N(CH ₃) ₂	8.40	1.01	0.43	2.76	7.29	1.76	
N(CH ₃) ₃	8.55	0.92	0.48	3.05	7.46	1.69	
NO ₂	8.36	1.18	0.55	2.40	7.47	1.48	
OH	8.17	1.09	0.49	2.71	7.40	1.74	
OCH ₃	8.30	1.03	0.44	2.94	7.36	1.76	
F	8.36	1.07	0.43	2.74	7.47	1.82 ^b	

^a ⁴J(1, CH₃) -0.75
⁵J(2, CH₃) 0.36
⁶J(3, CH₃) -0.62

^b ³J(1, F) 8.91
⁴J(2, F) 5.69
⁵J(3, F) 0.22

Substituent Effect S(*i,j*) for J_{HH} in Monosubstituted Benzenes

pos. <i>i,j</i>	F	Cl	Br	I	NO ₂	OCH ₃
1,2	+0.81	+0.61	+0.53	+0.39	+0.77	+0.79
1,3	-0.34	-0.23	-0.27	-0.25	-0.20	-0.32
1,4	-0.24	-0.16	-0.20	-0.19	-0.16	-0.22
1,5	+1.21	+0.87	-0.71	+0.51	+1.02	+1.33
2,3	-0.04	+0.03	-0.05	-0.04	-0.07	-0.16
2,4	+0.39	+0.34	+0.36	+0.37	+0.08	+0.38

Typical Stray Field Data for NMR Magnet Systems

Magnet System ¹ H MHz/mm Bore	Axial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line	Radial Distance (m) from Magnet Center to 5 Gauss (0.5 mT) Line
200 MHz/154 mm US PLUS LH	1.80	0.90
300 MHz/54 mm US LH	0.90	0.60
300 MHz/54 mm Fourier US LH	0.90	0.60
300 MHz/54 mm Ascend ULH	0.90	0.60
300 MHz/89 mm Ascend	1.10	0.55
300 MHz/154 mm US PLUS LH	2.00	1.00
400 MHz/54 mm Ascend	1.00	0.50
400 MHz/54 mm Ascend ULH	1.00	0.50
400 MHz/54 mm Ascend RS	1.00	0.50
400 MHz/89 mm Ascend	1.20	0.60
400 MHz/89 mm Ascend DNP	1.50	1.10
400 MHz/154 mm US PLUS LH	2.55	1.50
500 MHz/54 mm Ascend	1.20	0.60
500 MHz/54 mm Ascend ULH	1.20	0.60
500 MHz/54 mm Ascend RS	1.20	0.60
500 MHz/89 mm Ascend	1.20	0.60
500 MHz/154 mm US PLUS LH	2.55	1.50
600 MHz/54 mm Ascend	1.40	0.70
600 MHz/54 mm Ascend ULH	1.40	0.70
600 MHz/89 mm Ascend	2.00	1.00
600 MHz/89 mm Ascend DNP	2.00	1.00
700 MHz/54 mm Ascend	1.60	0.80
750 MHz/54 mm Ascend	2.00	1.00
750 MHz/89 mm Ascend	2.80	1.40
800 MHz/54 mm Ascend	2.50	1.50
850 MHz/54 mm Ascend	2.70	1.60
850 MHz/89 mm US ² WB	4.60	3.30
900 MHz/54 mm US ²	4.60	3.30
900 MHz/89 mm US ² WB	4.60	3.30
950 MHz/54 mm US ²	4.60	3.30
1000 MHz/54 mm UltraStabilized	15.00	12.00

LH = Long Hold, ULH = Ultra Long Hold

Abbreviations and Acronyms Used in Magnetic Resonance

2D	Two-Dimensional	BLEW-<i>n</i>	Burum-Linder-Ernst Windowless homonuc. dipolar dec. sequence of <i>n</i> pulses	CONOESY	Combined COSY/NOESY
3D	Three-Dimensional	BMS	Bulk Magnetic Susceptibility	CORMA	C omplete R elaxation M atrix A nalysis
ACCORDION	2D technique, simultaneous incrementing of evolution and mixing times	BOLD	Blood Oxygenation Level-Dependent contrast (MRI)	CORY-<i>n</i>	C ORY modification of BR-<i>n</i>
ADA	Alternated Delay Acquisition	BOSS	Bimodal Slice-Selective	COSS	C ORrelation with S hift S caling
ADC	Analog-to-Digital Converter, Apparent Diffusion Constant	BP	BiPhasic	COSY	C ORrelated S pectroscopy
ADEQUATE	Astonishingly Sensitive Double Quantum Transfer Experiment	BPP	Bloembergen/Purcell/Pound (theory)	COSY-45	COSY with 45° mixing pulse
ADLF	Adiabatic Demagnetization in the Laboratory Frame	BR-<i>n</i>	Burum-Rhim homonuclear dipolar decoupling sequence of <i>n</i> pulses	COSYDEC	COSY with F ₁ DEC oupling
ADRF	Adiabatic Demagnetization in the Rotating Frame	BSP	Bloch-Siegert Phase	COSYLR	COSY for Long-Range couplings
A.E.COSY	Alternative Exclusive COSY	BURP	Band-selective Uniform Response Pure-phase pulse	CP	C ross P olarization, C ircular P olarization
AFP	Adiabatic Fast Passage	bTFE	balanced Turbo Field Echo	CPD	Composite-Pulse Decoupling
AHT	Average Hamiltonian Theory	BW	BandWidth	CPMAS	C ross P olarization M agic-Angle S pinning
AJCP	Adiabatic J Cross Polarization	BWR	Bloch-Wangsness-Redfield theory	CPMG	C arr- P urcell- M eiboom- G ill Sequence
AMCP	Amplitude-Modulated Cross Polarization	CA	Contrast Agent	CRAMPS	Combined R otation A nd M ultiple P ulse S pectroscopy
ANGIO	MR ANGIO graphy	CAMELSPIN	Cross-relaxation Appropriate for Minimolecules Emulated by Locked SPINs	CRAZED	Correlated Spectroscopy Revamped by Asymmetric Z -gradient E cho D etection
APHH-CP	Adiabatic-Passage Hartmann-Hahn Cross Polarization	CBCA(CO)NH	Cβ(i,-1) and Cα(i,-1) , N(i) , H_N(i) 3D correl.	CRINEPT	C ross-correlated R elaxation-enhanced I NEPT
APT	Attached Proton Test	CBCANH	Cβ(i,-1) and Cα(i,-1) , N(i) , H_N(i) 3D correl.	CS	Contiguous S lice
AQ	Acquisition	CCPPA	Coupled Cluster Polarization Propagator Approximation	CSA	C hemical S hift A nisotropy
ARP	Adiabatic Rapid Passage	CE	Contrast-Enhanced	CSCM	C hemical S hift C orrelation M ap
ASIS	Aromatic Solvent-Induced Shift	CEST	Chemical Exchange Saturation Transfer	CSI	C hemical S hift I maging
ASL	Arterial Spin Labeling	CH-COSY	Carbon-Hydrogen C ORrelation S pectroscopy	CT	Constant T ime
ASTM	American Society for Testing and Materials	CHESS	C HEmical S hift S elective I maging S equence	CW	Continuous W ave
BASE	B asis imaging with S Elective-inversion preparation	CHIRP	rf pulse with linear freq. modulation	CYCLCROP	CYCL ic C ROSS P olarization
BB	BroadBand, as in decoupling	CIDEP	Chemically Induced Dynamic Electron Polarization	CYCLOPS	CYCL ically O rdered P hase S equence
BDR	Broadband Dipolar Recoupling	CIDNP	Chemically Induced Dynamic Nuclear Polarization	CYCLPOT	CYCL ic P OLarization T ransfer
bEPI	blipped EPI	CINE	"movie-like" MRI	DAC	Digital-to- A nalog C onverter
bFFE	balanced Fast-Field Echo	CISS	Constructive Interference Steady State	DAISY	D irect A ssignment I nter-connection S pectroscopy
BIRD	B ilinear R otation D ecoupling	CNR	Contrast-to- N oise R atio	DANTE	D elay A lternating with N utation for T ailored E xcitation
BIRD/2	half BIRD , bilinear $\pi/2$ pulse	COLOC	C ORrelated S pectroscopy via L ONG-Range C oupling	DAS	D ynamic A ngle S pinning
BLEW	A windowless multiple-pulse decoupling sequence	COLOC-S	COLOC with S uppression of one-bond correlations	DCNMR	N MR in Presence of an E lectric D irect C urrent
				DD	D ipole- D ipole
				DE	D ual E cho, D riven E quilibrium

Abbreviations and Acronyms Used in Magnetic Resonance

DECSY	D ouble- q uantum E cho C orrelated S pectroscop Y	DRAMA	D ipolar R ecovery A t the M agic A ngle	FA	F lip A ngle
DEFT	D riven E quilibrium F ourier T ransform	DREAM	D ouble-quantum R elay E nhancement by A diabatic M ixing	FADE	F ASE Acq. with D ouble E cho
DEPT	D istortionless E nhancement by P olarization T ransfer	DRESS	D epth R ESolved S pectroscopy	FAIR	F low-sensitive A lternating I nversion R ecovery
DEPTH	spin-echo sequence for spatial localization	DRIVE	DR iven E quilibrium	FASE	F ast A dvanced S pin E cho
DEPTQ	DEPT including quaternary carbons	DRYCLEAN	D iffusion- R educed water signals in spectroscop Y of mole C ules moving s L ow E r th A N water	FAST	F ourier- A cquired S TEady S tate
DFT	D iscrete F ourier T ransformation	DSA	D ata- S hift A cquisition	FASTMAP	F AST B_0 F ield M APping for shimming
DICE	D irect C onnectivity E xperiment	DSC	D ynamic S usceptibility C ontrast	FATE	F AsT T urbo E cho
DICOM	D igital I maging and C o M unications in M edicine	DSE	D ual S pin E cho	FC	F low C ompensation
DIGGER	D iscreet I solation from G radient- G overned E limination of R esonances	DTI	D iffusion T ensor I maging	FC2D_ANGIO	F low- C ompensated time-of-flight 2D A NGIO G raphy
DIPSI	Composite-pulse D ecoupling I n the P resence of S calar I nteractions	DTRCF	D ouble T ilted R otating C oordinate F rame	FE	F ield E cho, F requency E ncoding
DISCO	D ifferences and S ums within C OSY	DTSE	D ouble T urbo S pin E cho	FFE	F ast F ield E cho
DLB	D ifferential L ine B roadening	DUMBO	D ecoupling U sing M ind- B oggling O ptimization – a numerically optimized phase-modulated homonuc. dipolar dec. sequence	FFLG	F lip- F lop L ee- G oldburg decoupling
DNMR	D ynamic N M R	DWI	D iffusion- W eighted I maging	FFT	F ast F ourier T ransform
D.NOESY	D irect cross-relaxation NOESY	E-BURP	E xcitation BURP pulse	FGRE	F ast G radient- R ecalled E cho
DNP	D ynamic N uclear P olarization	EC	E ddy C urrents	FID	F ree I nduction D ecay
DOC	D ouble C onstant-Time sequence	E.COSY	E xclusive C orrelation S pectroscop Y	FIDS	F itting of D oublets and S inglets
DOPT	D ipolar O rder P olarization T ransfer	ECO-WURST	WURST decoupling with E limination of C ycling O scillations	FieldMap	B_0 F ield M apping for localized shimming
DOR	D ouble- O rientation R otation	EFG	E lectric F ield G radient	FIRFT	F ast I nversion- R ecovery F ourier T ransform
DOSY	D iffusion- O rdered S pectroscop Y	EM	E xponential M ultiplication	FISP	F ast I maging with S teady-state P recession
DOUBTFUL	D ouble Q uantum T ransition for F inding U nresolved L ines	EMF	E lectro M agnetic F ield E lectro M otive F orce	FL2D_ANGIO	F low-sensitive 2D A NGIO G raphy
DPFGSE	D ouble P ulsed F ield G radient S pin E cho	ENDOR	E lectron- N uclear D ouble R esonance	FLAIR	F Luid A ttenuation I nversion- R ecovery
DQ	D ouble Q uantum	ENMR	E lectrophoretic N M R	FLASH	F ast L ow- A ngle S HOT imaging
DQC	D ouble Q uantum C oherence	EPI	E cho- P lanar I maging	FLOCK	Long-range HETCOR using 3 BIRD pulses
DQF	D ouble Q uantum F ilter	EPR	E lectron P aramagnetic R esonance	FLOPSY	F lip- F IO P S pectroscop Y
DQF-COSY	D ouble Q uantum F iltered C OSY	EPS	E cho- P lanar S pectroscopy	FLOW_MAP	Q uantitative F LOW M APping and P C-angiography
DQSY	D ouble- Q uantum C OSY	ES, ESP	E cho S pacing	FMP	F ast M ulti P lanar
DQ/ZQ	D ouble Q uantum/ Z ero Q uantum S pectroscopy	E-SHORT	E nhanced S HORT repetition MRI	fMRI	f unctional M R I
		ESR	E lectron S pin R esonance	FOCSY	F oldover- C orrected S pectroscop Y
		E.TACS	E xclusive T ACS Y	FONAR	F ield-focusing M R I
		EXORCYCLE	4-step phase cycle for spin echoes	FOV	F ield O f V iew
		EXSY	E Xchange S pectroscop Y	FPT	F inite P erturbation T heory
				FR	F requency E ncoding
				FS	F at S aturation, F ast S can

Abbreviations and Acronyms Used in Magnetic Resonance

FSE	F ast S pin E cho	HCANNH	Hα(i) , Cα(i) , N(i) , H$_N$(i) 3D correl.	HORROR	double-quantum H o- n uclear R o- t ary R esonance
FSLG	F requency- S witched L ee- G oldburg – a homonuc. dipolar dec. scheme	(H)CC(CO) NH	Cα,β,...(i) , N(i+1) , H$_N$(i+1) 3D correl.	HQOC	H eteronuclear Q uadruple- Q uantum C orrelation
FSPGR	F ast S poiled G radient E cho	HCCH-COSY	Hα(i) , Cα(i) , Hβ(i) 3D correl.	HR	H igh R esolution
FT	F ourier T ransform	HCCH- TOCSY	total correlation of side- chain H and C	HRPA	H igher R andom P hase A pproximation
FUCOUP	F ully C OUpled S pectroscopy	HDQC	H eteronuclear D ouble- Q uantum C orrelation	HS	H omo S poil
FWHM	F ull (line) W idth at H alf M aximum	HEED	H ahn spin- E cho E xtende D sequence	HSL	H eteronuclear S pin L ock
GARP	G lobally O ptimized A lter- ing P hase R ectangular P ulses	HET2DJ	H ETeronuclear 2D J -correlated	HSQC	H eteronuclear S ingle- Q uantum C oherence
GE	G radient E cho	HETCOR	H ETeronuclear C ORrelation S pectroscopy	HTQC	H eteronuclear T riple- Q uantum C orrelation
GEFC	G radient E cho with F low C ompensation	HETLOC	H ETeronuclear L ONG-range C ouplings	I-BURP	I nversion BURP pulse
gem-COSY	g eminal-filtered COSY	HEHAHA	H ETeronuclear H ARTmann H Ahn	ICE	I ndirect C onnectivity E xperiment
GES	G radient- E cho S pectroscopy	HMBC	H eteronuclear M ultiple- B ond C orrelation	IDESS	I mproved D Epth S elective single surface coil S pectroscopy
GFE	G radient F ield E cho	HMQ	H eteronuclear M ultiple- Q uantum	IDR	I nverted D irect R esponse
GRASE	G RAient and S pin E cho	HMQC	H eteronuclear M ultiple- Q uantum C oherence	IEPI	I nterleaved EPI
GRASP	G RAient- A ccelerated S pectroscopy	HMSC	H eteronuclear M ultiple- and S ingle-bond C orrelation	IFT	I nverse FT
GRASS	G radient- R ecalled A cquisi- tion in the S teady S tate	HNCA	H$_N$(i) , N(i) , Cα(i) and Cα(i-1) 3D shift correlation	IGLO	I ndividual G auge for different L ocalized O rbitals
GRE	G radient- R ecalled E cho	HNCA-J	3D HNCA to measure ³ J(H _N ,H α)	INADE- QUATE	I ncredibly N atural A bu- dance D ouble Q UANatum T ransfer E xperiment
GRECCO	G RAient- E nhanced C arbon C oupling	HN(CA)NNH	H$_N$(i) , N(i) , N(i+1) and N(i-1) 3D correl.	INAPT	I NEPT with selective 1H excitation
GROESY	G radient- E nhanced S elective 1D ROESY	HN(CA)CO	H$_N$(i) , N(i) , C'O(i) , and C'O(i-1) 3D shift corre- lation	INDOR	I nternuclear D ouble R esonance
GROPE	G eneralized compensation for R esonance O ffset and P ulse length E rrors	H(N)CACO	H$_N$(i) , Cα(i) , C'O(i) 3D shift correlation	INEPT	I nsensitive N uclei E nhanced by P olarization T ransfer
GS	G radient S pectroscopy	HN(CA)CA	H$_N$(i) , N(i) , C'O(i-1) 3D shift correlation	INEPT+	I NEPT with refocusing peri- od for in-phase multiplets
gs- ...	g radient-selected ... (e.g. gs-COSY)	HNCAHA	H$_N$(i) , N(i) , Cα(i) , Hα(i) 4D shift correlation	INEPT-R	I NEPT R efocused for 1H- dec. spectra
H,X-COSY	H,X shift correlation (X-detected)	HNCO	H$_N$(i) , N(i) , C'O(i-1) 3D shift correlation	INSIPID	I nadequate S ensitivity I mprovement by P roton I ndirect D etection
HASTE	H alf- F ourier A cquisition S ingle-shot T urbo spin E cho	HN(CO)CA	H$_N$(i) , N(i) , Cα(i-1) 3D shift correlation	IntraGate- FLASH	C ardiac and respiration cine MRI with retrospec- tive (trigger-free) gating
HBHA (CBCA CO) NH	Hβ(i-1) and Hα(i-1) , N(i) , H$_N$(i) 3D correl.	H(N)COCA	H$_N$(i+1) , C'O(i) , Cα(i) 3D shift correlation	INVERSE	H , X correlation via ¹ H detection
HCACO	Hα(i) , Cα(i) , C'O(i) 3D correl.	HN(CO) CAHA	H$_N$(i+1) , N(i+1) , Cα(i) , Hα(i) 4D shift correlation	IPAP	I n- P hase A nti- P hase (in 2D)
HCACON	Hα(i) , Cα(i) , C'O(i) , N(i+1) 4D correl.	HOESY	H eteronuclear O verhauser E ffect S pectroscopy	IR	I nversion- R ecovery
HCA(CO)N	Hα(i) , Cα(i) , N(i+1) 3D correl.	HOHAHA	H omonuclear H ARTmann- H Ahn S pectroscopy	IRMA	I terative R elaxation M atrix A nalysis
HCA(CO) NNH	Hα(i) , Cα(i) , N(i+1) , H$_N$(i+1) 4D correl.			ISECR	I n-pha S E C Ross peaks (method)

Abbreviations and Acronyms Used in Magnetic Resonance

ISIS	Image-Selected In-vivo Spectroscopy (single-voxel)	MGE	Multiple Gradient Echo	MSOFT	MultiSlice Off-resonance FaT Suppression
IST	Irreducible Spherical Tensor	MINIP	MINimum Intensity Projection	MSP	Multiple Sensitive Point
IVIM	IntraVoxel Incoherent Motion	MIP	Maximum Intensity Projection	MSPGSE	Multiple-Stepped PGSE
JCP	J Cross-Polarization	MLEV	M. Levitt's CPD sequence	MT	Magnetization Transfer
J-mod	J modulation	MLM	Maximum Likelihood Method	MTC	Magnetization Transfer Contrast
JR	Jump-and-Return sequence (90, - τ -90 _y)	MOTSA	Multiple Overlapping Thin Slab(Slice) Acquisition	MTSA	Multiple Thin-Slab Acquisition
J-res	J-resolved 2D	MP	Multiple Pulse, MultiPlanar, Magnetization-Prepared	MUSIC	MUltiplicity-Selective In-phase Coherence transfer
LAS	Laboratory Axis System	MPF_n	Multiple-Pulse Decoupling with Phase and Frequency Switching with <i>n</i> offsets	MVS	Multiple Volume Spectroscopy
LASE	Low-Angle SE	MP-GR	MultiPlanar Gradient-Recalled Acq. in Steady State	NEDOR	Nuclear Electronic DOuble Resonance
LB	Line Broadening (via EM)	MPR	MultiPlanar Reconstruction	NERO	Nonlinear Excitation with Rejection on Resonance
LG	Lorentz-Gauss window function	MP-RAGE	Magnetization-Prepared RApid Gradient Echo (MP-GRE)	NEWS	Narrow-gap non-Excitation for Water Suppression
LIS	Lanthanide Induced Shift	MQ	Multiple-Quantum	NEX	Number of EXcitations
LORG	Local ORIGIN	MQC	Multiple-Quantum Coherence	NMR	Nuclear Magnetic Resonance
LOSY	LOcalized SpectroscopY	MQF	Multiple-Quantum Filter	NOE	Nuclear Overhauser Effect
LP	Linear Polarization, Linear Prediction	MQHPT	Multiple-Quantum Heteronuclear Polarization Transfer	NOE-DIFF	NOE-DIFFerence spectroscopy
LPSVD	Linear Prediction using Singular Value Decomposition	MQS	Multiple-Quantum Spectroscopy	NOESY	NOE-based 2D shift correlation
LSR	Lanthanide Shift Reagent	MR	Magnetic Resonance	NOVEL	Nuclear Orientation Via Electron spin Locking
LUT	LookUp Table	MRA	MR Angiography	NPW	No Phase Wrap
MAGROFI	MAGnetization Grid ROTating-Frame Imaging	MREV-<i>n</i>	Mansfield-Rhim-Elleman-Vaughan homonuc. dipolar dec. cycle of <i>n</i> pulses	NQCC	Nuclear Quadrupole Coupling Constant
MARCO POLO	Multiple Analysis by Reduction of Cross peaks and Ordering of Patterns in an Overdetermined Library Organization	MRV	MR Venography	NQR	Nuclear Quadrupole Resonance
MARDI-GRAS	Matrix Analysis of Relaxation for DIstance GeometRY of an Aqueous STructure	MRI	Magnetic Resonance Imaging	NQS	Non-Quaternary Suppression
MARF	Magic Angle in the Rotating Frame	MRS	Magnetic Resonance Spectroscopy	NSPECT	Non-localized SPECTroscopy
MAS	Magic-Angle Spinning	MRSI	Magnetic Resonance Spectroscopic Imaging	OBTUSE	Offset Binomial Tailored for Uniform Spectral Excitation
MASS	Magic-Angle Sample Spinning	MRT	Magnetic Resonance Tomography	OCS	Optimized Cosine-Sine pulse
MAST	Motion Artifact Suppression Technique	MS	MultiSlice	ODMR	Optically Detected Magnetic Resonance
MDEFT	Modified Driven Equilibrium FT method	mSENSE	modified SENSE	OS	Overcontiguous Slices
ME	MultiEcho	MS-EPI	MultiShot EPI	OSIRIS	Outer-Volume-Suppressed Image-Related In vivo Spectroscopy – a modification of ISIS
MEDUSA	Technique for the Determination of Dynamic Structures	MSHOT-<i>n</i>	Magic Sandwich High-Order Truncation homonuc. dipolar decoupling sequence with <i>n</i> TREV-4 sandwiches	PACE	Prospective Acquisition CorrEction
MEM	Maximum Entropy Method	MSME	MultiSlice MultiEcho (T2 mapping)	PAR	Phase-Alternated Rotation of magnetization
MEMP	MultiEcho MultiPlanar				
MESS	MultiEcho Single Shot				
MFISP	Mirrored FISP (PSIF)				

Abbreviations and Acronyms Used in Magnetic Resonance

PARACEST	PARA magnetic C hemical E xchange S aturation T ransfer	PRFT	P artially R elaxed F ourier T ransform	RELAY	RELAY ed C orrelation S pectroscopy
PAS	P rincipal A xis S ystem	PROPELLER	P eriodically R otated O verlapping P arallel L ines with E nhanced R econstruction	REPAY	R everse E ditng of P rotons A ccording to multiplicit Y
PC	P hase C ontrast	PS	P artial S aturation	REREDOR	R otor- E ncoded REDOR
PCA	P hase C ontrast A ngio-graphy	PS-COSY	P hase- S ensitive COSY	REST	R Egional S aturation T echnique
PCOSY	P urged COSY	PSD	P hase- S ensitive D etection	RF	R adio F requency
PD	P roton D ensity	PSIF	mirrored FISP (SE acquisition)	RFDR	RF - D riven R ecoupling
PDLF	P roton- D etected L ocal F ield	PT	P olarization T ransfer	RF-FAST	RF -spoiled FAST
PE	P hase E ncoding	PW	P ulse W idth	RFOV	R ectangular FOV
PE.COSY	P rimitive E.COSY , P urged E xclusive COSY	PWI	P erfusion- W eighted I maging	RICE	R apid I maging using C omposite E cho
PEDRI	P roton- E lectron D ouble R esonance I maging	Q	Q uality F actor (of RF coil/circuit) Q uantitative ... (e.g. QMRI , QCSI)	RIDE	R ing D own E limination
PELF	P roton- E ncoded L ocal F ield	QF	Q uadrupole moment/ F ield gradient (interaction or relaxation mechanism)	RINEPT	R everse INEPT
PENDANT	P olarization E nhancement D uring A ttached N ucleus T esting	Q Flow	Q uantification	RISE	R apid I maging using S pin E cho
PEP	P reservation of E quivalent P athways	QPD	Q uadrature P hase D etection	RMSD	R oot- M ean- S quare D eviation
PFG	P ulsed F ield G radient	QUEST	Q Uick E cho S plit I maging T echnique	ROAST	R esonant O ffset A veraging in the S Teady S tate
PFGSE	P ulsed F ield G radient S pin E cho	QUIPSS	Q Uantitative I maging of P erfusion using a S ingle S ubtraction	RODI	R OTatin- g rame r elaxation D ispersion I maging
PGSE	P ulsed G radient S pin E cho	RAM	R apid A cquisition M atrix	ROE	R otating-frame O verhauser E ffect
PISEMA	P olarization I nversion with S pin E xchange at the M agic A ngle	RARE	R apid A cquisition R elaxation E nhanced	ROESY	ROE -based 2D shift correlation
PITANSEMA	P olarization I nversion T ime A veraged N utation S pin E xchange at the M agic A ngle	RAREst	R ARE with s hort tE using s lew-rate-optimized gradients	ROI	R egion O f I nterest
PJR	P ower-adapted J ump and R eturn	RAREVTR	R ARE with V ariable TR (simultaneous T_1 & T_2 mapping)	ROPE	R espiratory O rded PE
PMFG	P ulsed M agnetic F ield G radient	RASE	R apid A cquisition S pin E cho	ROTO	ROESY - TO CSY R elay
PMLG	P hase- M odulated L ee- G oldburg dipolar decoupling	RBW	R eciever B and W idth	RPA	R andom P hase A pproximation
PMRFI	P hase- M odulated R otating- F rame I maging	RCF	R otating C oordinate F rame	RR	R otational R esonance
POF	P roduct O perator F ormalism	RCT	R elayed C oherence T ransfer	RSSARGE	RF - S poiled SARGE
POMMIE	P hase O scillations to M axi M ize E ditng	RE	R apid E xcitation (MRI)	RT	R espiratory T rigger
POST	P ermutationally O ffset- S Tabilized	REAPDOR	R otational E cho A diabatic P assage D ouble R esonance	RUFIS	R otating U ltra F ast I maging S equence
PRE	P roton R elaxation E nhancement	RE-BURP	R efocused B and-selective U niform R esponse P ure phase	SA	S hielding A nisotropy
Presat	P resaturation (usually of solvent)	RECSY	M ultistep R elayed C oherence S pectroscop Y	SAR	S pecific A bsorption R ate (RF)
PRESS	P oint- R ESolved S pectroscopy	REDOR	R otational E cho D ouble R esonance	SARGE	S poiled steady-state A cquisition with R ewinded G radient E cho

Abbreviations and Acronyms Used in Magnetic Resonance

SDDS	Spin Decoupling Difference Spectroscopy	SINGLE PULSE	SINGLE PULSE -acquire spectroscopy	SR	Saturation-Recovery
SDEPT	Selective DEPT	SIS	Substituent-Induced Shift	SRP	Self-Refocusing Pulse
SE	Spin Echo	SJR	Second-order Jump and Return	SS	Slice Selection (gradient), Single Slice
SECSY	Spin-Echo Correlated SpectroscopY	SKEWSY	SKEW ed Exchange SpectroscopY	SSB	Shifted Sine-Bell window function
SEDOR	Spin-Echo DO uble R esonance	SL	Spin-Lock pulse	SSFP	Steady-State Free Precession
SEDRA	Simple Excitation for Dephasing of Rotational echo Amplitudes	SLF	Separated Local Field	SSFSE	Single-Shot FSE
SEDUCE	SE lective D ecoupling U sing C rafted E xcitation	SLITDRESS	SL ice in T erleaved D ePTH R ESolved S urface coil S pectroscopy	SSI	Solid State Imaging
SEFT	Spin-Echo Fourier Transform Spectroscopy (with J modulation)	SLOPT	Spin-L ocking P olarization T ransfer	SSMP	Single-Slice Multiple-Phase
SELCOSY	SE lective COSY	SMART	Shimadzu Motion Artifact Reduction Technique	ssNMR	solid-state NMR
SELTICS	Sideband EL imination by T emporary I nterruption of the C hemical S hift	SMASH	Short Minimum Angle SH ot, S imultaneous A cquisition of S patial H armonics	SSTSE/T2	Single-Shot TSE with T2 weighting
SELINCOR	SE lective I Nverse COR relation	SNR or S/N	Signal-to-Noise Ratio	ST	Saturation Transfer, Slice Thickness
SELINQUATE	SE lective I NADEQUATE	SOPPA	Second-Order Polarization Propagator Approach	STAGE	Small Tip Angle GE
SELRESOLV	SE lective R ESolution of C,H Coupling	SORS/STC	Slice-selective Off-Resonance Sinc Pulse / Saturation Transfer Contrast	STE	ST imulated E cho
SEMS	Spin-Echo MultiSlice	SPACE	S PATial and C hemical-Shift E ncoded E xcitation	STEAM	ST imulated E cho A cquisition M ode for imaging
SEMUT	Subspectral Editing Using a MULTIPLE-Quantum Trap	SPAIR	S Pectral S election A ttenuated I nversion R ecoverY	STEP	STE Progressive I maging
SENSE	SENS itivity E ncoding	SPECIFIC-CP	S PECtrally I nduced F iltering I n C ombination with C ross P olarization	STERF	Steady-State T echnique with R efocused F ID
sEPI	spiral EPI	SPEED	Swap Phase-Encoded Data	STIR	Short T1 Inversion-Recovery
SEPT	Selective INEPT	SPGR	S Poiled G radient- R ecalled	STREAM	S uppressed T issue with R efreshment A ngiography M ethod
SERF	SE lective R e F ocussing	SPI	Selective Population Inversion	STUD	Sech/Tanh Universal Decoupling – an adiabatic decoupling scheme
SESAM	SE mi- S elective A cquisition M odulated (Decoupling)	SPIDER	Steady-state Projection Imaging with Dynamic Echo Train Readout	SUBMERGE	S Uppression B y M istuned E cho and R epeatitive G radient E pisodes
SFAM	Simultaneous Freq. and Ampl. Modulation	SPIO	SuperParamagnetic Iron Oxide	SUSAN	Spin decoupling employing Ultra-broadband inversion sequences generated via Simulated AN ealing
SFORD	Single Frequency Off-Resonance Decoupling	SPIR	Spectral Presaturation Inversion-Recovery	SWATTR	Selective Water Attenuation by T2 and T1 Relaxation
SGSE	Steady-Gradient Spin-Echo	SPIRAL	MRI with SPIRAL k-space scan	SVS	Single-Volume Spectroscopy
SHECOR	Selective H eteronuclear COR relation	SPRITE	Single-Point Ramped Imaging with T1 Enhancement	T1 ...	T1-weighted ... (method)
SHORT	SHORT repetition techniques	SPT	Selective Population Transfer	T1W	T1-Weighted
SI	Spectroscopic Imaging	SQ	Single-Quantum	T2 ...	T2-weighted ... (method)
SIAM	Simultaneous acq. of In-phase and Antiphase Multiplets	SQC	Single-Quantum Coherence	T2W	T2-Weighted
SIP	Saturation Inversion Projection	SQF	Single-Quantum Filter	T2*W	T2*-Weighted
SIMBA	Selective Inverse Multiple-Bond Analysis			TACSY	T Aylored C orrelation S pectroscop Y
SINEPT	SINE -dependent PT			TANGO	Testing for Adjacent Nuclei with a Gyration Operator

Abbreviations and Acronyms Used in Magnetic Resonance

TART	Tip Angle Reduced T ₁ Imaging	TrueFISP	FISP with balanced gradient waveform	WFOP	Water Fat Opposed Phase
TD	Trigger Delay, Time Difference	TS	Time of Saturation	WFS	Water Fat Separation (Shift Difference)
TCF	Time Correlation Function	TSE	Turbo Spin Echo	WHH-<i>n</i>	WAHUHA dec. cycle of <i>n</i> pulses
TE	Time delay between excitation and Echo maximum	TSETSE	double-resonance Two-Spin Effect for correlation spectroscopy	WIM-<i>n</i>	Windowless Isotropic Mixing dec. cycle of <i>n</i> pulses
TEDOR	Transferred-Echo Double Resonance	TSR	Total SR	WURST	Wideband, Uniform Rate, and Smooth Truncation – an adiabatic decoupling sequence
TEI	TE Interleaved	Turbo-FLASH	FLASH sequence during one IR period	XCORFE	H, X CORrelation using a Fixed Evolution time
TF	Turbo Factor	U-BURP	Universal BURP pulse	XD-NOESY	eXchange-Decoupled NOESY
TFE	Turbo Field Echo	UE	Unpaired Electron (relaxation mechanism)	X-FILTER	Selection of ¹ H- ¹ H correlation when both H are coupled to X
TGSE	Turbo Gradient Spin Echo	UFSE	UltraFast SE	X-HALF-FILTER	Selection of ¹ H- ¹ H correlation when one H is coupled to X
THRIVE	T1W High-Resolution Isotropic Volume Examination	UNCOSY	UNiform excitation COSY	Z-COSY	Z-filtered COSY
TI	Time following Inversion	USPIO	UltraSmall Paramagnetic Iron Oxide	Z-FILTER	pulse sandwich for elimination of signal components with dispersive phase
TIR	Turbo IR	UTE	Ultra-short TE radial scan	ZECSY	Zero-Quantum-Echo Correlation Spectroscopy
TMR	Topical Magnetic Resonance	UTSE	Ultra-short TSE	ZIP	Zero-fill Interpolation Processing
TOBSY	TOTAL through-Bond correlation Spectroscopy	VAPRO	VARIABLE PROjection method	ZQ	Zero Quantum
TOCSY	TOTAL Correlation Spectroscopy	VAS	Variable Angle Spinning	ZQC	Zero-Quantum Coherence
TOF	Time-Of-Flight	VE	Velocity-Encoded	ZQF	Zero-Quantum Filter
TOE	Truncated NOE	VEC	Velocity-Encoded Cine (MRI)	ZZ-Spectroscopy	Selection of coherences involving ZZ or longitudinal two-spin order
TOPE	Tilt-Optimized Nonsaturated Excitation	VEMP	Variable-Echo MultiPlanar	ZZZ-Spectroscopy	Selection of coherences involving longitudinal 3-spin order
TORO	TOCSY-ROESY Relay	VENC	Velocity ENCoding value	β-COSY	COSY with low-angle mixing pulse
TOSS	TOTAL Suppression of Sidebands	VEST	Volume Excitation Stimulated echoes	Ψ-COSY	pseudo-COSY using incremented freq.-selective excitation
TPPI	Time-Proportional Phase Incrementation	VIGRE	Volumetric Interpolated GRAdient Echo		
TPPM	Two-Pulse Phase Modulation	VOI	Volume Of Interest		
TPR	Time and Phase Reversal	VOSING	VOLUME-selective Spectral editing		
TQ	Triple-Quantum	VOSY	VOLUME-Selective Spectroscopy		
TQF	Triple-Quantum Filter	VPS	Volumes Per Segment		
TR	Time for Repetition of excitation	VSOP	Very Small superparamagnetic iron Oxide Particles		
T/R	Transmit/Receive	WAHUHA	WAUGH-HUBER-HAEberlien Sequence		
TRAPDOR	TRANSFER of Populations in Double Resonance	WALTZ	CPD Sequence Containing the Elements 1-2-3		
TRCF	Tilted Rotating Coordinate Frame	WATER-GATE	WATER suppression through GRAdient Tailored Excitation		
TREV-<i>n</i>	Time-REVERSAL echo sequence of <i>n</i> pulses for homonuc. dipolar dec.	WATR	Water Attenuation by Transverse Relaxation		
TRNOE	TRANSFERRED NOE	WEFT	Water Eliminated Fourier Transform		
TROSY	Transverse Relaxation Optimized Spectroscopy	WET	Water suppression Enhanced through T1 effects		
T-ROESY	Transverse ROESY				

Symbols for NMR and Related Quantities*

Roman alphabet	
a or A	Hyperfine (electron-nucleus) coupling constant
$A_q^{(l,m)}$	The m th component of an irreducible tensor of order l representing the nuclear spin operator for an interaction of type q
\mathbf{B}	Magnetic field (strictly the magnetic flux density or magnetic induction)
\mathbf{B}_0	Static magnetic field of an NMR spectrometer
$\mathbf{B}_1, \mathbf{B}_2$	Radiofrequency magnetic fields associated with frequencies ν_1, ν_2
\mathbf{B}_l	Local magnetic field of random field or dipolar origin
\mathbf{C}	Spin-rotation interaction tensor
C_X	Spin-rotation coupling constant of nuclide X
\mathbf{D}	Dipolar interaction tensor
D_{ij}	Dipolar coupling constant between nuclei (i and j), in Hz
D^C	Nuclear receptivity relative to that of ^{13}C
D^P	Nuclear receptivity relative to that of ^1H
\mathbf{E}	Electric field strength
F	Spectral width
F_1, F_2 or f_1, f_2	The two frequency dimensions of a two-dimensional spectrum
\hat{F}_G	Nuclear spin operator for a group, G , of nuclei
F_G	Magnetic quantum number associated with \hat{F}_G
g	Nuclear or electronic g factor (Landé splitting factor)
G	Magnetic field gradient amplitude
\hat{H}	Hamiltonian operator
H_{ij}	Matrix element of Hamiltonian operator
\hat{I}_j	Nuclear spin operator for nucleus j
\hat{I}_+, \hat{I}_-	'Raising' and 'lowering' spin operators for nucleus j
I_j	Magnetic quantum number associated with \hat{I}_j
\mathbf{J}	Indirect coupling tensor
${}^nJ_{AB}$	Spin-spin coupling constant for nuclei A and B through n bonds in Hz
$J(\omega)$	Spectral density of fluctuations at angular frequency ω
${}^nK_{AB}$	Reduced nuclear spin-spin coupling constant $K_{AB} = 4\pi^2 J_{AB} / (h\gamma_A\gamma_B)$ in T^2J^{-1}

\mathbf{L}	Angular momentum
m_l	Eigenvalue of \hat{I}_z (magnetic component quantum number)
m_{tot}	Total magnetic component quantum number for a spin system (eigenvalue of $\sum \hat{I}_{z,i}$)
$m_{\text{tot}}(X)$	Total magnetic component quantum number for X -type nuclei
\mathbf{M}_0	Equilibrium macroscopic magnetization per unit volume in the presence of \mathbf{B}_0
M_x, M_y, M_z	Components of macroscopic magnetization per volume
M_n	n th moment of spectrum ($M_2 =$ second moment, etc.)
n_α, n_β	Populations of the α and β spin states
N	Total number of nuclei of a given type per unit volume in the sample
\mathbf{q}	Electric field gradient tensor in units of the elementary charge
eQ	Nuclear quadrupole moment, Q is in m^2 and e is the elementary charge in C
R_1^X	Spin-lattice (longitudinal) relaxation rate constant for nucleus X
R_2^X	Spin-spin (transverse) relaxation rate constant for nucleus X
R_{1p}^X	Longitudinal relaxation rate constant for nucleus X in the reference frame rotating with \mathbf{B}_1
S	Signal intensity
\hat{S}	Electron (or, occasionally, nuclear) spin operator; cf. \hat{I}
t_1, t_2	Time dimensions for two-dimensional NMR
T_c	Coalescence temperature under chem. exchange for signals in an NMR spectrum
T_1^X	Spin-lattice (longitudinal) relaxation time of the X nucleus
T_2^X	Spin-spin (transverse) relaxation time of the X nucleus
T_2	Net dephasing time for M_x or M_y
T_{1p}^X	Longitudinal relaxation time for the X nucleus in the reference frame rotating with \mathbf{B}_1
T_d	Pulse (recycle) delay
T_{ac}	Acquisition time
$T_q^{(l,m)}$	The m th component of an irreducible tensor of order l representing the strength of an interaction of type q

* IUPAC Recommendations: Magnetic Resonance in Chemistry, Vol. 36, 145-149 (1998)

Symbols for NMR and Related Quantities*

\mathbf{V}	Electric field gradient tensor. $\mathbf{V} = e\mathbf{q}$, where e is the elementary charge
$V_{\alpha\beta}$	Elements of Cartesian electric field gradient tensor
W_{0r}, W_1, W_2	Relaxation rate constants (transition probabilities per time) between energy levels differing by 0, 1 and 2 in m_{rot}
W_{rs}	Transition probability between spin states r and s
Greek alphabet	
α	Nuclear spin wavefunction (eigenfunction of \hat{I}_z) for the $m_i = +\frac{1}{2}$ state of a spin- $\frac{1}{2}$ nucleus
α_E	The Ernst angle (for optimum sensitivity)
β	Nuclear spin wavefunction (eigenfunction of \hat{I}_z) for the $m_i = -\frac{1}{2}$ state of a spin- $\frac{1}{2}$ nucleus
γ_X	Magnetogyric ratio of nucleus X
δ_X	Chemical shift (for the resonance) of nucleus of element X, usually in ppm
Δn	Population difference between nuclear states (Δn_0 at Boltzmann equilibrium)
$\Delta\delta$	Change or difference in δ
$\Delta\nu_{1/2}$	Full width in frequency units of a resonance line at half-height
$\Delta\sigma$	Anisotropy in σ [$\Delta\sigma = \sigma_{zz} - \frac{1}{2}(\sigma_{xx} + \sigma_{yy})$]
$\Delta\chi$	(i) Susceptibility anisotropy ($\Delta\chi = \chi_{ } - \chi_{\perp}$); (ii) difference in electronegativities
ϵ_0	Permittivity of the vacuum
ζ	Anisotropy in shielding, expressed as $\sigma_{zz} - \sigma_{iso}$
η	(i) Nuclear Overhauser enhancement; (ii) tensor asymmetry factor; (iii) viscosity
κ	Skew of a tensor
θ	Angle, especially for that between a given vector and \mathbf{B}_0
μ	(i) Magnetic dipole moment (component μ_z along \mathbf{B}_0); (ii) electric dipole moment
μ_0	Permeability of the vacuum
μ_B	Bohr magneton (earlier β_0)
μ_N	Nuclear magneton (earlier β_N)
ν_j	Larmor or resonance frequency of nucleus j (in Hz)
ν_0	(i) Spectrometer operating frequency; (ii) Basic Larmor or resonance frequency for a given isotope

ν_1	Frequency of primary RF magnetic field B_1 (excitation, detection)
ν_2	Frequency of secondary RF magnetic field B_2 (decoupling)
$\bar{\nu}_X$	Normalized resonance frequency for nucleus X relative to ν_H for tetramethylsilane (TMS) at the same \mathbf{B}_0 field; $\bar{\nu}_X = 100 \nu_X/\nu_H$ (TMS)
ρ	Density matrix
$\hat{\rho}$	Density operator
ρ_{ij}	Element of matrix representation of $\hat{\rho}$
σ	Shielding tensor
σ_j	(Isotropic) shielding constant of nucleus j
$\sigma_{ }, \sigma_{\perp}$	Components of shielding tensor σ parallel and perpendicular to the symmetry axis
$\hat{\sigma}$	Reduced density operator
τ	(i) Time between RF pulses or recovery time following inversion (ii) lifetime in dynamic NMR studies
τ_c	Correlation time for molecular motion, especially for isotropic molecular tumbling
τ_d	Dwell time for data sampling
τ_{null}	Recovery time leading to null M_z after a 180° pulse
τ_p	Pulse duration
τ_{sc}	Correlation time for relaxation by the scalar mechanism
τ_{sr}	Correlation time for spin-rotation relaxation
$\tau_{ }, \tau_{\perp}$	Correlation times for molecular tumbling parallel and perpendicular to the symmetry axis
χ	(i) Magnetic susceptibility; (ii) nuclear quadrupole coupling constant ($\chi = e^2 q_{zz} Q/h$)
$\omega, \omega_0, \omega_1, \omega_2$	As for ν , ν_0 , ν_1 , ν_2 but in angular frequency units (rad/s)
Ω	Span of a tensor
Ω_1, Ω_2	Angular frequency of RF fields $\mathbf{B}_1, \mathbf{B}_2$

* IUPAC Recommendations: *Magnetic Resonance in Chemistry*, Vol. 36, 145-149 (1998)

¹H Chemical Shifts for Common Contaminants in Deuterated Solvents

	Proton	mult., J	CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
residual solvent H			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H ₂ O		s	1.56	2.84 ^a	3.33 ^a	0.40	2.13	4.87	
acetic acid	CH ₃	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
acetone	CH ₃	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
acetonitrile	CH ₃	s	2.10	2.05	2.07	1.55	1.96	2.03	2.06
benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33	
<i>t</i> -butanol	CH ₃	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OH ^c	s			4.19	1.55	2.18		
<i>t</i> -butyl methyl ether	CCH ₃	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	OCH ₃	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
BHT ^b	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92	
	OH ^c	s	5.01		6.65	4.79	5.20		
	ArCH ₃	s	2.27	2.22	2.18	2.24	2.22	2.21	
	ArC(CH ₃) ₃	s	1.43	1.41	1.36	1.38	1.39	1.40	
chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90	
cyclohexane	CH ₂	s	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-dichloroethane	CH ₂	s	3.73	3.87	3.90	2.90	3.81	3.78	
dichloromethane	CH ₂	s	5.30	5.63	5.76	4.27	5.44	5.49	
diethyl ether	CH ₃	t, 7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	CH ₂	q, 7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
diglyme	CH ₂	m	3.65	3.56	3.51	3.46	3.53	3.61	3.67
	CH ₂	m	3.57	3.47	3.38	3.34	3.45	3.58	3.61
	OCH ₃	s	3.39	3.28	3.24	3.11	3.29	3.35	3.37
1,2-dimethoxyethane	CH ₃	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	CH ₂	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
dimethylacetamide	CH ₃ CO	s	2.09	1.97	1.96	1.60	1.97	2.07	2.08
	NCH ₃	s	3.02	3.00	2.94	2.57	2.96	3.31	3.06
	NCH ₃	s	2.94	2.83	2.78	2.05	2.83	2.92	2.90
dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97	7.92
	CH ₃	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	CH ₃	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
dimethylsulfoxide	CH ₃	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
dioxane	CH ₂	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
ethanol	CH ₃	t, 7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	CH ₂	q, 7 ^d	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s ^{c,d}	1.32	3.39	4.63		2.47		
ethyl acetate	CH ₃ CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH ₂ CH ₃	q, 7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH ₂ CH ₃	t, 7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	CH ₃ CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH ₂ CH ₃	q, 7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH ₂ CH ₃	t, 7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
ethylene glycol	CH	s ^e	3.76	3.28	3.34	3.41	3.51	3.59	3.65
"grease" ^f	CH ₃	m	0.86	0.87		0.92	0.86	0.88	
	CH ₂	br s	1.26	1.29		1.36	1.27	1.29	
<i>n</i> -hexane	CH ₃	t	0.88	0.88	0.86	0.89	0.89	0.90	
	CH ₂	m	1.26	1.28	1.25	1.24	1.28	1.29	
HMPA ^g	CH ₃	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64	2.61
methanol	CH ₃	s ^h	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s ^{c,h}	1.09	3.12	4.01		2.16		
nitromethane	CH ₃	s	4.33	4.43	4.42	2.94	4.31	4.34	4.40
<i>n</i> -pentane	CH ₃	t, 7	0.88	0.88	0.86	0.87	0.89	0.90	
	CH ₂	m	1.27	1.27	1.27	1.23	1.29	1.29	

¹H Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

	Proton	mult.	CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
<i>i</i> -propanol	CH ₃	d, 6	1.22	1.10	1.04	0.95	1.09	1.50	1.17
	CH	sep, 6	4.04	3.90	3.78	3.67	3.87	3.92	4.02
pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53	8.52
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44	7.45
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85	7.87
silicone grease ⁱ	CH ₃	s	0.07	0.13		0.29	0.08	0.10	
tetrahydrofuran	CH ₂	m	1.85	1.79	1.76	1.40	1.80	1.87	1.88
	CH ₂ O	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
toluene	CH ₃	s	2.36	2.32	2.30	2.11	2.33	2.32	
	CH(<i>α/p</i>)	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH(<i>m</i>)	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3	7.16	
triethylamine	CH ₃	t, 7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	CH ₂	q, 7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

^a In these solvents the intermolecular rate of exchange is slow enough that a peak due to HDO is usually also observed; it appears at 2.81 and 3.30 ppm in acetone and DMSO, respectively. In the former solvent, it is often seen as a 1:1:1 triplet, with ²J_{H,D} = 1 Hz.

^b 2,6-di-*tert*-butyl-4-methylphenol. ^c The signals from exchangeable protons were not always identified. ^d In some cases (see note *a*), the coupling interaction between the CH₂ and the OH protons may be observed (*J* = 5 Hz). ^e In CD₃CN, the OH proton was seen as a multiplet at δ = 2.69, and extra coupling was also apparent on the methylene peak. ^f Long-chain, linear aliphatic hydrocarbons. Their solubility in DMSO was too low to give visible peaks. ^g Hexamethylphosphoramide. ^h In some cases (see notes *a*, *d*), the coupling interaction between the CH₃ and the OH protons may be observed (*J* = 5.5 Hz). ⁱ Poly(dimethylsiloxane). Its solubility in DMSO was too low to give visible peaks.

¹³C Chemical Shifts for Common Contaminants in Deuterated Solvents

		CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
solvent signals		77.16	29.84	39.52	128.06	1.32	49.00	
			206.26			118.26		
acetic acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH ₃	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH ₃	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH ₃	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
<i>t</i> -butanol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH ₃	31.25	30.72	30.38	30.47	30.68	30.91	30.29
<i>t</i> -butyl methyl ether	OCH ₃	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH ₃	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH ₃ Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH ₃ C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH ₂	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dichloroethane	CH ₂	43.50	45.25	45.02	43.59	45.54	45.11	
dichloromethane	CH ₂	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH ₃	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH ₂	65.91	66.12	62.05	65.94	66.32	66.88	66.42

¹³C Chemical Shifts for Common Contaminants in Deuterated Solvents (continued)

		CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
diglyme	CH ₃	59.01	58.77	57.98	58.66	58.90	59.06	58.67
	CH ₂	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH ₂	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH ₃	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH ₂	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH ₃	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH ₃	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH ₃	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH ₃	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH ₃	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH ₃	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH ₂	67.14	67.60	66.36	67.16	67.72	68.11	67.19
ethanol	CH ₃	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH ₂	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH ₃ CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH ₂	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH ₃	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH ₃ CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH ₂ CH ₃	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH ₂ CH ₃	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH ₂	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH ₂	29.76	30.73	29.20	30.21	30.86	31.29	
<i>n</i> -hexane	CH ₃	14.14	14.34	13.88	14.32	14.43	14.45	
	CH ₂ (2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH ₂ (3)	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA ^b	CH ₃	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH ₃	50.41	49.77	48.59	49.97	49.90	49.86	49.50 ^c
nitromethane	CH ₃	62.50	63.21	63.28	61.16	63.66	63.08	63.22
<i>n</i> -pentane	CH ₃	14.08	14.29	13.28	14.25	14.37	14.39	
	CH ₂ (2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH ₂ (3)	34.16	34.83	33.48	34.45	34.89	35.30	
<i>i</i> -propanol	CH ₃	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH ₃	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH ₂	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH ₂ O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH ₃	21.46	21.46	20.99	21.10	21.50	21.50	
	C(<i>i</i>)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(<i>o</i>)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(<i>m</i>)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(<i>p</i>)	125.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH ₃	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH ₂	46.25	47.07	45.74	46.77	47.10	46.96	47.19

^a See footnotes for Table 1. ^b ²J_{FC} = 3 Hz. ^c Reference material; see text.

Quantity	Formula (bold face = vectors)	Definitions (SI units) (see SI section for constants and units)
Magnetic Field Magnetic Force	$\mathbf{B} = \mu_0 \mathbf{H}$ $\mathbf{F} = Q \mathbf{v} \times \mathbf{B}$	\mathbf{B} = magn. flux density, magn. induction (T) \mathbf{H} = magn. field strength (A m ⁻¹) μ_0 = permeability of vacuum ($4\pi \times 10^{-7}$ H m ⁻¹) Q = elec. charge (C); v = velocity (m/s)
Nuclear Spin Spin Angular Mom. Magn. Moment	\mathbf{I} $\hbar m_l$ $\boldsymbol{\mu}_l = \gamma_l \hbar \mathbf{I} = g_l \beta_N \mathbf{I}$	γ = magnetogyric ratio (rad s ⁻¹ T ⁻¹); $\hbar = h/2\pi$ $\beta_N = \mu_B$ (nuclear magneton); g_l = nuclear g factor m_l = quantum no. ($-l, -l+1, \dots, +l$)
Zeeman Interaction Larmor Freq. Nutation Vector	$\mathbb{H} = -\boldsymbol{\mu}_l \cdot \mathbf{B}_0, E = -m_l \gamma_l \hbar B_0$ $\omega_0 = \gamma_l B_0, \nu_0 = \gamma_l B_0$ $\boldsymbol{\omega} = -\gamma_l \mathbf{B}$	ω in rad s ⁻¹ , ν in Hz ($\Delta m_l = \pm 1$), $\gamma = \gamma/2\pi$ (clockwise precession in lab frame for $\gamma > 0$)
Boltzmann Pop. Diff. Equil. Magn.	$\Delta N/N \sim \gamma_l \hbar/2kT$ ($\Delta m_l = \pm 1$) $M_0 = B_0 [N\gamma^2 \hbar^2 l(l+1) / 3kT]$	N = number of nuclei with spin l T = temperature (K)
Rotating Frame (r.f.) and residual field	$\gamma \Delta \mathbf{B}_0 = \gamma \mathbf{B}_0 + \boldsymbol{\omega}_{r.f.}$ $\boldsymbol{\Omega} = -\gamma \Delta \mathbf{B}_0 = \boldsymbol{\omega}_0 - \boldsymbol{\omega}_{r.f.}$	$\boldsymbol{\omega}_{r.f.}$ = rot. frame vector (detector freq.) in direction $\boldsymbol{\omega}_0$ (-z axis for $\gamma > 0$) $\Delta \mathbf{B}_0$ = residual field in r.f. $\boldsymbol{\Omega}$ = precession freq. in r.f. (clockwise in r.f. for $\omega_0 > \omega_{r.f.}$)
Effective RF Field Amplitude and Tilt Nutation	$\omega_1 = -\gamma \mathbf{B}_1, \mathbf{B}_{eff} = \mathbf{B}_1 + \Delta \mathbf{B}_0$ $B_{eff} = [B_1^2 + \Delta B_0^2]^{1/2}, \tan \theta = \Delta B_0/B_1$ β_{eff} (in rad) = $-\gamma \mathbf{B}_{eff} \tau_p$ γB_{eff} (in Hz) = $1/(4\tau_{90})$	\mathbf{B}_1 = RF field vector in xy plane; nutation is ccw around $\boldsymbol{\omega}_{eff} = -\gamma \mathbf{B}_{eff}$; θ = tilt angle between \mathbf{B}_{eff} and xy -plane; for $\Delta B_0/B_1 < 0.1$: $\theta < 6^\circ$, $B_{eff} \approx B_1$ τ_p = RF pulse width (s); $\tau_{90} = 90^\circ$ pulse
Optimum flip angle	$\cos \beta_{opt} = \exp(-TR/T_1)$	TR = pulse repetition time
Relaxation rates	spin-lattice: $R_1 = 1/T_1$ spin-spin: $R_2 = 1/T_2 = \pi \Delta \nu_0$	$\Delta \nu_0$ = natural Lorentzian linewidth at half-height
Bulk Susceptibility Correction	for cylindrical samples with external ref. in coaxial capillary $\delta_{corr} = \delta_{obs} + C (\chi_{ref} - \chi_{sample})$	$C = +2\pi/3$ (tube perpendicular to B_0) $C = -4\pi/3$ (tube parallel to B_0)
Spin-echo amplitude in constant B_0 gradient	$M(2\tau) = M_0 \exp[-2\tau/T_2 - (2/3)(\gamma G)^2 D\tau^3]$	90- τ -180- τ Hahn echo with gradient G D = diffusion coeff. in gradient direction
Spin-echo attenuation in PFG-SE experiment	$\ln(S_{echo}/S_0) = -bD$ $b = (\gamma \delta G)^2 (\Delta - \delta/3)$	$G = B_0$ gradient pulse amplitude (T/m) δ = pulse width; Δ = pulse spacing
Rotational Correlation Time	Stokes-Einstein Relation $\tau_c = (4\pi \eta r^3) / (3kT)$	τ_c = rot. correlation time for isotropic tumbling η = viscosity; r = molecular radius (sphere)
Nuclear Oberhauser Enhancement	$M_S(I)/M_S(0) = 1 + 0.5(\gamma_I/\gamma_S)(R_1^{IS}/R_1^S)$ (extreme narrowing; $\omega_S \tau_c \ll 1$)	enhancement of spin S due to continuous irradiation of spin I ; R_1^{IS} = dipolar relaxation of S via I ; R_1^S = relaxation of S via all mechanisms
Polarization Transfer	$M_S(PT)/M_S(0) = \gamma_I/\gamma_S$	PT from I to S via J_{IS}
Lorentzian Lineshape	$a(\omega) = R_2 / [R_2^2 + \Delta\omega^2]$ $d(\omega) = \Delta\omega / [R_2^2 + \Delta\omega^2]$	$a(\omega), d(\omega)$ = absorption, dispersion signals $\Delta\omega = \omega - \Omega$

NMR Relaxation

Mechanisms (isotropic tumbling, SI units)	Remarks
<p>Intramolecular Heteronuclear Dipole-Dipole</p> <p>Spin I relaxed by Spin S</p> $R_1^I = E_{IS} r_{IS}^{-6} [(1/12)J_0(\omega_I - \omega_S) + (3/2)J_1(\omega_I) + (3/4)J_2(\omega_I + \omega_S)]$ $R_2^I = E_{IS} r_{IS}^{-6} [(1/6)J_0(0) + (1/24)J_0(\omega_I - \omega_S) + (3/4)J_1(\omega_I) + (3/2)J_1(\omega_S) + (3/8)J_2(\omega_I + \omega_S)]$ <p>where $E_{IS} = (\mu_0/4\pi)^2 (\gamma_I \gamma_S \hbar)^2 S(S+1)$</p> <p>Extreme narrowing: $R_1^I = (4/3) E_{IS} r_{IS}^{-6} \tau_c (\omega\tau_c \ll 1)$</p> <p>For several spins S: use $\sum r_{IS}^{-6}$</p> <p>NB: $T_1^I = 1/R_1^I$ only when S is saturated</p>	<p>Factor $(\mu_0/4\pi) = 10^{-7}$ is required for conversion from cgs-Gauss units to MKSA (SI) units.</p> <p>Spectral Densities for random isotropic rotation</p> $J_q(\omega) = C_q [\tau_c / (1 + \omega^2 \tau_c^2)]$ <p>($q = 0, 1, 2$)</p> <p>$C_0 = 24/15$; $C_1 = 4/15$; $C_2 = 16/15$</p> <p>extreme narrowing: $J_q(\omega) = C_q \tau_c$</p>
<p>Intramolecular Homonuclear Dipole-Dipole</p> <p>Spin I_k relaxed by Spin I_l</p> $R_1^I = E_l r_{kl}^{-6} (3/2) [J_1(\omega_l) + J_2(2\omega_l)]$ $R_{1p}^I = E_l r_{kl}^{-6} [(3/8)J_0(\omega_l) + (15/4)J_1(\omega_l) + (3/8)J_2(2\omega_l)]$ $R_2^I = E_l r_{kl}^{-6} [(3/8)J_0(0) + (15/4)J_1(\omega_l) + (3/8)J_2(2\omega_l)]$ <p>where $E_l = (\mu_0/4\pi)^2 \gamma_l^4 \hbar^2 l(l+1)$</p> <p>Extreme narrowing: $R_1^I = R_2^I = 2 E_l r_{kl}^{-6} \tau_c (\omega\tau_c \ll 1)$</p> <p>For several spins l: use $\sum r_{kl}^{-6}$</p>	
<p>Intermolecular Heteronuclear Dipole-Dipole</p> <p>Spin I on mol. A relaxed by Spin S on mol. B ($\omega\tau_c \ll 1$)</p> $R_1^I = 16\pi c_S E_{IS} / (27 r_{IS} D_{trans})$ <p>(pair distribution function = step function)</p>	<p>$E_{IS} = (\mu_0/4\pi)^2 (\gamma_I \gamma_S \hbar)^2 S(S+1)$</p> <p>$c_S$ = conc. of spins S</p> <p>r_{IS} = distance of closest approach</p> $D_{trans} = (D_A + D_B) / 2$
<p>Intermolecular Homonuclear Dipole-Dipole</p> <p>Spin I on mol. A relaxed by Spin I on mol. B ($\omega\tau_c \ll 1$)</p> $R_1^I = 8\pi c_l E_l / (9 r_{ll} D_{trans})$ <p>also found in the literature is:</p> $R_1^I = (4\pi/3) c_l E_l (\tau/r_{ll}^3) [1 + (2r_{ll}^2/5 D_{trans} \tau)]$	<p>$E_l = (\mu_0/4\pi)^2 \gamma_l^4 \hbar^2 l(l+1)$</p> <p>$c_l$ = conc. of spins l</p> <p>r_{ll} = distance of closest approach</p> <p>τ = mol. jump time</p>

Spherical Harmonics

Spherical harmonics up to rank 2 expressed in polar and orthogonal Cartesian coordinates

$Y_{0,0}$	=	$\sqrt{\frac{1}{4\pi}}$	
$Y_{1,0}$	=	$\sqrt{\frac{3}{4\pi}} \cos \theta$	= $\sqrt{\frac{3}{4\pi}} \frac{z}{r}$
$Y_{1,\pm 1}$	=	$\mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$	= $\mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$
$Y_{2,0}$	=	$\sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$	= $\sqrt{\frac{5}{16\pi}} \frac{2z^2 - x^2 - y^2}{r^2}$
$Y_{2,\pm 1}$	=	$\mp \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta e^{\pm i\phi}$	= $\mp \sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$
$Y_{2,\pm 2}$	=	$\sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}$	= $\sqrt{\frac{15}{32\pi}} \frac{(x \pm iy)^2}{r^2}$

Mechanisms (isotropic tumbling, SI units)	Remarks
<p>Chemical Shift Anisotropy (CSA)</p> <p>molecular tumbling modulates the interaction of the chem. shift tensor with the B_0 field.</p> $R_1 = (2/5) E_{CSA} [\tau_c / (1 + \omega^2 \tau_c^2)]$ $R_2 = (1/90) E_{CSA} \{8\tau_c + [6\tau_c + (1 + \omega^2 \tau_c^2)]\}$	<p>predominant relaxation mech. for non-protonated X nuclei</p> $E_{CSA} = \gamma^2 B_0^2 \Delta\sigma^2$ $\Delta\sigma = \sigma_{\perp} - \sigma_{\parallel} \text{ (in ppm)}$ <p>(assuming axial symmetry of tensor)</p>
<p>Quadrupole Relaxation ($I > 1/2$)</p> $R_1 = R_2 = (3/40) C_1 [1 + \eta^2/3] C_{QF}^2 \tau_c \quad (\omega\tau_c \ll 1)$	$C_1 = (2I + 3) / [I^2(2I - 1)]$ $C_{QF} = e^2 Q q_{zz} / \hbar = \text{quadrupolar coupling in Hz; } \eta = \text{asymmetry param.}$
<p>Spin-Rotation Interaction (SR)</p> <p>Relaxation arises from the interaction of the nuclear spin with magnetic fields generated by the rotation of a molecular magnetic moment modulated by molecular collisions:</p> $\left(\frac{1}{T_1}\right)_{SR} = \frac{2 \hbar kT}{3 \hbar^2} C_{eff}^2 \tau_J$ <p>i = moment of inertia of the molecule C_{eff} = effective spin-rotational coupling constant τ_J = angular momentum correlation time</p> <p>With $\tau_c \cdot \tau_J = \frac{i}{6kT}$, we can introduce the reorientational correlation time and we obtain:</p> $\left(\frac{1}{T_1}\right)_{SR} = \frac{R_i}{9 \hbar^2} C_{eff}^2 \cdot \frac{1}{\tau_c}$	
<p>Scalar Coupling (SC)</p> <p>This relaxation mechanism can occur if the nucleus I in question is scalar coupled (with coupling constant J) to a second spin ($S \geq 1/2$) and the coupling is modulated by either chemical exchange (SC relaxation of the first kind) or the relaxation of spin S, e.g. if $S > 1/2$, (SC relaxation of the second kind). In this case spin splittings disappear and single lines are observed.</p> $\left(\frac{1}{T_1}\right)_{SC} = \frac{8\pi^2 J^2 S(S+1)}{3} \left[\frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2 \tau_{SC}^2} \right]$ $\left(\frac{1}{T_2}\right)_{SC} = \frac{4\pi^2 J^2 S(S+1)}{3} \left[\tau_{SC} + \frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2 \tau_{SC}^2} \right]$ <p>$\tau_{SC} = \tau_e$, if exchange time $\tau_e \ll T_1$ of either spin (first kind) $\tau_{SC} = T_1^S$ (the relaxation time of spin S) if $T_1^S \ll \tau_e, 1/2\pi J$ (second kind)</p> <p>ω_I and ω_S are the resonance of I and S at the magnetic field in which $\left(\frac{1}{T_{1,2}}\right)_{SC}$ is measured.</p>	