NMR Solvent Data Chart

Cambridge Isotope Labs

The ¹H spectra of the residual protons and ¹³C spectra were obtained on a Varian Gemini 200 spectrometer at 295°K. The sample for the proton and ¹³C spectra contain a maximum of 0.05% and 1.0% TMS (v/v) respectively. Since deuterium has a spin of 1, triplets arising from coupling to deuterium have the intensity ratio of 1:1:1. 'm' denotes a broad peak with some fine structures. It should be noted that the chemical shifts, in particular, can be dependent on solute, concentration and temperature.

□ Approximate values only, may vary with pH, concentration and temperature.

Melting and boiling points are those of the corresponding unlabeled compound (except for D_2O). These temperature limits can be used as a guide to determine the useful liquid range of the solvents.

SOLVENT	¹H Chemical Shift (ppm from TMS) (multiplicity)	JHD (Hz)	Carbon-13 Chemical Shift (ppm from TMS) (multiplicity)	JCD (Hz)	¹H Chemical Shift of HOD □ (ppm from TMS)	Density at 20°C	Melting point (°C)	Boiling point (°C)	Dielectric Constant	Molecular Weight
Acetic Acid-d_4	11.65 (1) 2.04 (5)	 2.2	178.99 (1) 20.0 (7)	 2.0	11.5	1.12	17	118	6.1	64.08
Acetone-d_6	 2.05 (5)	 2.2	206.68 (13) 29.92 (7)	0.9 19.4	2.8	0.87	-94	57	20.7	64.12
Acetonitrile-d_3	 1.94 (5)	 2.5	118.69 (1) 1.39 (7)	 21	2.1	0.84	-45	82	37.5	44.07
Benzene-d_6	7.16 (1)		128.39 (3)	24.3	0.4	0.95	5	80	2.3	84.15
Chloroform-d	7.27 (1)		77.23 (3)	32.0	1.5	1.50	-64	62	4.8	120.38
Cyclohexane-d_{12}	1.38 (1)		26.43 (5)	19	0.8	0.89	6	81	2.0	96.24
Deuterium Oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.8	101.4	78.5	20.03
N, N-Dimethyl -formamide-d_7	8.03 (1) 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	3.5	1.04	-61	153	36.7	80.14
Dimethyl Sulfoxide-d_6	2.50 (5)	1.9	39.51 (7)	21.0	3.3	1.18	18	189	46.7	84.17
1,4-Dioxane-d_8	3.53 (m)		66.66 (5)	21.9	2.4	1.13	12	101	2.2	96.16
Ethanol-d_6	5.29 (1) 3.56 (1) 1.11 (m)		 56.96 (5) 17.31 (7)	 22 19	5.3	0.89	<-130	79	24.5	52.11
Methanol-d_4	4.87 (1) 3.31 (5)	 1.7	 49.15 (7)	 21.4	4.9	0.89	-98	65	32.7	36.07
Methylene Chloride-d_2	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	40		86.95
Pyridine-d_5	8.74 (1) 7.58 (1) 7.22 (1)		150.35 (3) 135.91 (3) 123.87 (5)	27.5 24.5 25	5	1.05	-42	116	12.4	84.13
Tetrahydrofuran-d_8	3.58 (1) 1.73 (1)		67.57 (5) 25.37 (1)	22.2 20.2	2.4-2.5	0.99	-109	66	7.6	80.16
Toluene-d_8	 7.09 (m) 7.00 (1) 6.98 (5) 2.09 (5)	 2.3	137.86 (1) 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	 23 24 24 19	0.4	0.94	-95	111	2.4	100.19
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4) 116.6 (4)		11.5	1.50	-15	72		115.03
Trifluoroethanol-d_3	5.02 (1) 3.88 (4x3)	 2(9)	126.3 (4) 61.5 (4X5)	 22	5	1.45	-44	75		103.06

CIL

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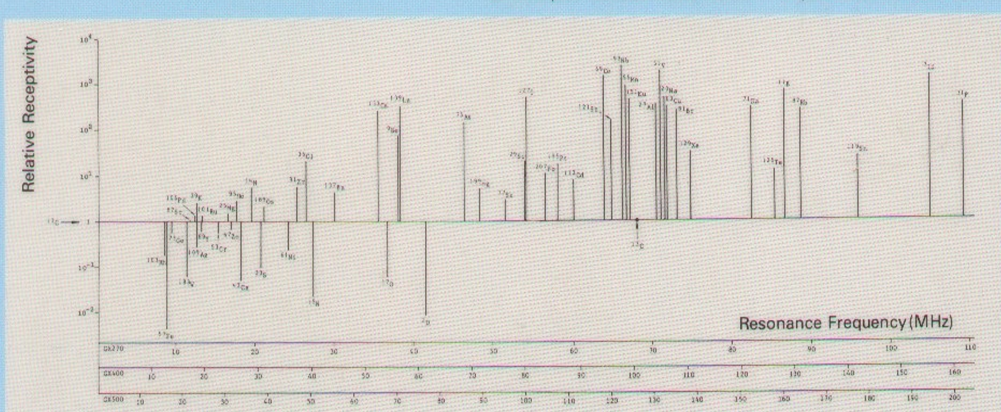
NMR Observation Frequencies for GX-series

Isotope	Observation Frequency			Natural Abundance	Spin(I)	Relative Sensitivity
	GX270	GX400	GX500			
※ 1H	270.166	399.782	500.125	99.985	1/2	1.00
2D	41.472	61.369	76.773	1.5×10^{-2}	1	9.65×10^{-3}
3T	288.168	426.420	533.449		1/2	1.21
6Li	39.758	58.832	73.598	7.42	1	8.50×10^{-3}
※ 7Li	105.014	155.396	194.400	92.58	3/2	0.293
9Be	37.962	56.175	70.275	100	−3/2	1.39×10^{-2}
10B	29.032	42.960	53.743	19.58	3	1.99×10^{-2}
※ 11B	86.677	128.262	160.455	80.42	3/2	0.165
※ 13C	67.938	100.533	125.766	1.108	1/2	1.59×10^{-2}
※ 14N	19.519	28.884	36.134	99.63	1	1.01×10^{-3}
※ 15N	27.379	40.514	50.683	0.37	−1/2	1.04×10^{-3}
※ 17O	36.634	54.210	67.817	3.7×10^{-2}	−5/2	2.91×10^{-2}
※ 19F	254.191	376.142	470.552	100	1/2	0.833
※ 23Na	71.458	105.742	132.282	100	3/2	9.25×10^{-2}
※ 25Mg	16.538	24.472	30.615	−10.13	−5/2	2.67×10^{-3}
※ 27Al	70.396	104.169	130.315	100	5/2	0.206
※ 29Si	53.674	79.426	99.361	4.70	−1/2	7.84×10^{-2}
※ 31P	109.381	161.858	202.483	100	1/2	6.63×10^{-2}
※ 33S	21.039	31.133	38.948	0.76	3/2	2.26×10^{-3}
※ 35Cl	26.471	39.170	49.002	75.53	3/2	4.70×10^{-3}
37Cl	22.032	32.602	40.785	24.47	3/2	2.71×10^{-3}
39K	12.606	18.654	23.336	93.10	3/2	5.08×10^{-4}
41K	6.919	10.238	12.808	6.88	3/2	8.40×10^{-5}
※ 43Ca	17.911	26.504	33.156	0.145	−7/2	6.40×10^{-3}
45Sc	65.631	97.119	121.495	100	7/2	0.301
47Ti	15.229	22.536	28.192	7.28	−5/2	2.09×10^{-3}
49Ti	15.232	22.540	28.197	5.51	−7/2	3.76×10^{-3}
50V	26.936	39.858	49.862	0.24	6	5.55×10^{-2}
51V	71.008	105.075	131.448	99.76	7/2	0.383
53Cr	15.270	22.596	28.267	9.55	−3/2	9.03×10^{-4}
55Mn	66.634	98.602	123.351	100	5/2	0.175
57Fe	8.729	12.917	16.159	2.19	1/2	3.37×10^{-5}
※ 59Co	64.106	94.862	118.672	100	7/2	0.277
61Ni	24.142	35.724	44.691	1.19	−3/2	3.57×10^{-3}
※ 63Cu	71.607	105.961	132.557	69.09	3/2	9.31×10^{-2}
65Cu	76.711	113.514	142.005	30.91	3/2	0.114
67Zn	16.899	25.006	31.283	4.11	5/2	2.85×10^{-3}
69Ga	64.840	95.948	120.030	60.4	3/2	6.91×10^{-2}
※ 71Ga	82.387	121.914	152.514	39.6	3/2	0.142
73Ge	9.423	13.944	17.444	7.76	−9/2	1.40×10^{-3}
※ 75As	46.281	68.484	85.673	100	3/2	2.51×10^{-2}
※ 77Se	51.525	76.245	95.382	7.58	1/2	6.93×10^{-3}
79Br	67.687	100.161	125.301	50.54	3/2	7.86×10^{-2}
※ 81Br	72.980	107.993	135.099	49.46	3/2	9.85×10^{-2}
83Kr	10.393	15.380	19.240	11.55	−9/2	1.88×10^{-3}
85Rb	26.085	38.599	48.287	72.15	5/2	1.05×10^{-2}
※ 87Rb	88.403	130.815	163.649	27.85	3/2	0.175
87Sr	11.706	17.323	21.670	7.02	−9/2	2.69×10^{-3}
89Y	13.235	19.585	24.501	100	−1/2	1.18×10^{-4}
91Zr	25.206	37.300	46.662	11.23	−5/2	9.48×10^{-3}
※ 93Nb	66.036	97.717	122.244	100	9/2	0.482
95Mo	17.061	26.046	32.583	15.72	5/2	3.23×10^{-3}
97Mo	17.971	26.593	33.268	9.46	−5/2	3.43×10^{-3}
99Ru	9.133	13.515	16.907	12.72	−3/2	1.95×10^{-4}
101Ru	13.241	19.594	24.511	17.07	−5/2	1.41×10^{-3}
103Rh	8.505	12.585	15.744	100	−1/2	3.11×10^{-5}
105Pd	12.371	18.306	22.901	22.23	−5/2	1.12×10^{-3}
107Ag	10.934	16.179	20.240	51.82	−1/2	6.62×10^{-5}
109Ag	12.568	18.598	23.266	48.18	−1/2	1.01×10^{-4}
111Cd	57.286	84.770	106.047	12.75	−1/2	9.54×10^{-3}
※113Cd	59.926	88.676	110.933	12.26	−1/2	1.09×10^{-2}
113In	59.069	87.408	109.347	4.28	9/2	0.345
115In	59.204	87.608	109.597	95.72	9/2	0.342
115Sn	88.342	130.725	163.536	0.35	−1/2	3.50×10^{-2}
117Sn	96.249	142.426	178.175	7.61	−1/2	4.52×10^{-2}
※119Sn	100.682	148.985	186.380	8.58	−1/2	5.18×10^{-2}
121Sb	64.653	95.672	119.685	57.25	5/2	0.160
123Sb	98.467	145.708	182.281	42.75	7/2	4.57×10^{-2}
123Te	70.812	104.785	131.086	0.87	−1/2	1.80×10^{-2}
125Te	85.348	126.295	157.994	6.99	−1/2	3.15×10^{-2}
※127I	54.062	79.999	100.078	100	5/2	9.34×10^{-2}
129Xe	74.731	110.584	138.340	26.44	1/2	2.12×10^{-2}
※133Cs	35.443	52.448	65.612	100	7/2	4.74×10^{-2}
135Ba	26.838	39.714	49.682	6.59	3/2	4.90×10^{-3}
137Ba	30.024	44.428	55.579	11.32	3/2	6.86×10^{-3}
139La	38.164	56.473	70.648	99.911	7/2	5.92×10^{-2}
141Pr	79.459	117.581	147.094	100	5/2	0.293
143Nd	14.689	21.736	27.192	12.17	−7/2	3.38×10^{-3}
145Nd	9.024	13.353	16.704	8.3	−7/2	7.86×10^{-4}
147Sm	11.158	16.511	20.655	14.97	−7/2	1.48×10^{-3}
149Sm	8.890	13.156	16.457	13.83	−7/2	7.47×10^{-4}
151Eu	66.990	99.130	124.011	47.82	5/2	0.178
153Eu	29.589	43.784	54.774	52.18	5/2	1.53×10^{-2}
155Gd	10.253	15.172	18.980	14.73	−3/2	2.79×10^{-4}
159Tb	61.315	90.731	113.504	100	3/2	5.83×10^{-2}
161Dy	8.904	13.175	16.482	18.88	−5/2	4.17×10^{-4}
163Dy	12.681	18.765	23.475	24.97	5/2	1.12×10^{-3}
165Ho	55.379	81.948	102.516	100	7/2	0.181
167Er	7.825	11.578	14.485	22.94	−7/2	5.07×10^{-4}
169Tm	22.327	33.039	41.331	100	−1/2	5.66×10^{-4}
171Yb	47.584	70.414	88.087	14.31	1/2	5.46×10^{-3}
173Yb	13.108	19.397	24.266	16.13	−5/2	1.33×10^{-3}
175Lu	30.826	45.615	57.064	97.41	7/2	3.12×10^{-2}
177Hf	8.375	12.393	15.504	18.5	7/2	6.38×10^{-4}
179Hf	5.126	7.586	9.490	13.75	−9/2	2.16×10^{-4}
181Ta	32.337	47.851	59.861	99.988	7/2	3.60×10^{-2}
183W	11.242	16.635	20.810	14.40	1/2	7.20×10^{-5}
185Re	60.825	90.007	112.598	37.07	5/2	0.133
187Re	61.449	90.930	113.753	62.93	5/2	0.137
187Os	6.222	9.207	11.518	1.64	1/2	1.22×10^{-5}
189Os	21.051	31.151	38.970	16.1	3/2	2.34×10^{-3}
191Ir	4.644	6.872	8.597	37.3	3/2	2.53×10^{-5}
193Ir	5.055	7.480	9.357	62.7	3/2	3.27×10^{-5}
※195Pt	58.077	85.941	107.511	33.8	1/2	9.94×10^{-3}
197Au	4.625	6.844	8.562	100	3/2	2.51×10^{-5}
※199Hg	48.308	71.484	89.426	16.84	1/2	5.67×10^{-3}
201Hg	17.831	26.386	33.008	13.22	−3/2	1.44×10^{-3}
203Tl	154.400	228.475	285.821	29.50	1/2	0.187
205Tl	155.910	230.710	288.617	70.50	1/2	0.192
※207Pb	56.534	83.657	104.655	22.6	1/2	9.16×10^{-3}
209Bi	43.416	64.245	80.370	100	9/2	0.137
235U	4.863	7.196	9.002	0.7205	7/2	1.21×10^{-4}

※Isotopes whose observation frequencies are stored on GX standard software.



Relative Receptivity based on ^{13}C

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Table of Isotopes and NMR Parameters

Isotope (The shaded ones are of spin I=1/2)

- Mass number
- Relative receptivity* (^{13}C=1.0)
- Chemical shift range (in ppm)

Example: C — 13 — 1.0 — 200

Li 6 7 3.58 1.5×10^{3} 10	Be 9 79 40		H 1 2 5.7×10^{3} 8.2×10^{-3} 10	H 3 6.9×10^{3} 10								B 10 11 22 754 150	C 13 1.0 200	N 14 15 5.7 2.2×10^{-2} 900	O 17 6.1×10^{-2} 1600	F 19 4.7×10^{3} 200	Ne 21
Na 23 525 30	Mg 25 1.5 40											Al 27 117 400	Si 29 2.1 400	P 31 377 600	S 33 9.7×10^{-2} 1000	Cl 35 37 2.2 3.8 1000	Ar
K 39 41 2.7 3.3×10^{-2} 30	Ca 43 5.27×10^{-2} 70	Sc 45 1.7×10^{3} 350	Ti 47 49 8.7×10^{-1} 1.18 1700	V 50 51 7.5×10^{-1} 2150 2400	Cr 53 0.49 2000	Mn 55 994 3000	Fe 57 4.2×10^{-3} 3000	Co 59 1570 18000	Ni 61 0.24 100	Cu 63 65 365 201 600	Zn 67 0.665 300	Ga 69 71 237 319 1000	Ge 73 0.617 1100	As 75 143 800	Se 77 3.0 2000	Br 79 81 226 277 500	Kr 83 123
Rb 85 87 43 277 200	Sr 87 1.1 60	Y 89 0.668 600	Zr 91 6.04	Nb 93 2740 2200	Mo 95 97 2.9 1.8 5500	Tc 99 2134 3000	Ru 99 101 8.3×10^{-1} 1.56 8300	Rh 103 0.18 6000	Pd 105 1.41	Ag 107 109 0.2 0.28 600	Cd 111 113 6.9 7.6 800	In 113 115 84 1.9×10^{3} 1100	Sn 117 119 20 25 2700	Sb 121 123 520 111 3500	Te 123 125 8.9×10^{-1} 13 4000	I 127 530 4000	Xe 129 32 7000
Cs 133 269 300	Ba 135 137 1.8 4.4 10	La 139 3.4×10^{2} 300	Hf 177 179 8.8×10^{-1} 0.27	Ta 181 2.0×10^{2}	W 183 6.0×10^{-2} 6900	Re 185 187 2.8×10^{2} 4.9×10^{2}	Os 187 189 1.1×10^{-3} 2.1	Ir 191 193 2.0×10^{-2} 0.05	Pt 195 19 15000	Au 197 0.06	Hg 199 201 5.4 1.1 3000	Tl 203 205 2.89×10^{2} 770 7000	Pb 207 12 3500	Bi 209 777	Po	At	Rn
			Ce	Pr 141 1.7×10^{5}	Nd 143 145 233 37	Pm	Sm 147 149 125 59	Eu 151 153 4.8×10^{4} 4.5×10^{3}	Gd 155 157 23 52	Tb 159 3.3×10^{4}	Dy 161 163 45 16	Ho 165 1.0×10^{5}	Er 167 66	Tm 169 3.2	Yb 171 173 4.1 1.14	Lu 175 156	

* *Relative Receptivity = Natural abundance × Relative sensitivity*

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The elements in orange areas play an important role in the living system.